A COMPUTER PROGRAM FOR EVALUATING LATTICE SUMS

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by

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B.S., Oregon State University, 1958

Submitted in partial fulfillment
for the degree of

MASTER OF SCIENCE IN PHYSICS

from the

UNITED STATES NAVAL POSTGRADUATE SCHOOL

May 1966

ABSTRACT

A recurring problem in solid state physics is that of determining the electrostatic field or potential at a point within the crystal lattice arising from the molecules of the lattice themselves. A typical problem is that of finding the electrostatic binding potential of an ionic lattice, assuming point changes.

Nijboer, de Wette and others have worked toward perfecting a method for calculating the electric field arising from a lattice of dipoles. This work culminated in a paper by de Wette and Schacher detailing a procedure which ensures a rapidly converging summation of the three dimensional lattice sums involved.

The present paper is an extension of the latter, presenting a computer program for evaluating dipole fields in a crystal lattice using the equations obtained by de Wette and Schacher.

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BACKGROUND

A recurring problem in solid state physics is that of determining the electrostatic field or potential at a point within the crystal lattice arising from the molecules of the lattice themselves. A typical problem is that of finding the electrostatic binding potential of an ionic lattice, assuming point changes.

Nijboer, de Wette[1,2] and others have worked toward perfecting a method for calculating the electric field arising from a lattice of dipoles. This work culminated in a paper by de Wette and Schacher[3] detailing a procedure which ensures a rapidly converging summation of the three dimensional lattice sums involved.

The present paper is an extension of the latter, presenting a computer program for evaluating dipole fields in a crystal lattice using the equations obtained by de Wette and Schacher.

[1] B.R.A. Nijboer and F.W. de Wette, Physica 14, 422 (1958)

[2] F.W. de Wette, Phys. Rev. 123, 103 (1961)

[3] F.W. de Wette and G.E. Schacher, Phys. Rev. 137, A78 (1965)

THEORY[4]

Virtually all problems concerning crystal self fields reduce ultimately to evaluating a lattice sum of the general form:

$$S(\underline{x},\underline{y},\underline{z}) = \sum_{a,b,c=-\infty}^{+\infty} f(\underline{x}-a\underline{a}_1, \underline{y}-b\underline{a}_2, \underline{z}-c\underline{a}_3)$$

where $\underline{x}$, $\underline{y}$, and $\underline{z}$ are coordinates of the point at which the sum is to be evaluated; f ( ) represents the contribution to the sum from a particular lattice point; and $a\underline{a}_1$, $b\underline{a}_2$, $c\underline{a}_3$ are the coordinates of the lattice points whose contribution is being considered ($\underline{a}_1$, $\underline{a}_2$, and $\underline{a}_3$ being lattice basis vectors).

Finding the electric field due to a lattice of dipoles reduces to evaluating such a sum, where the summation is, mathematically, conditionally convergent. That is, the value of the sum depends on the order in which the summation is carried out (analagous to the fact that the internal field of a crystal depends on the shape of the crystal). Thus, any procedure for evaluating dipole sums must, at some point, make an assumption of a particular crystal shape.

[4]For a complete description see (2)

In the procedure used here these conditionally convergent triple sums over the real lattice are converted into absolutely (rapidly) convergent double sums over the recipricol lattice. Converting from a triple to a double sum forces an assumption of a slab-shaped crystal with the short dimension in the z-direction (perpendicular to the plane described by the lattice vectors $\underline{a}_1$ and $\underline{a}_2$. See figure 1 for relations between x, y, z coordinates and the lattice basis vectors).

To achieve the conversion to an absolutely convergent double sum, the original sum is first Fourier transformed, making use of the property of lattice sums that the summation of a function over a lattice in real space is equal to the sum of its Fourier transform over the recipricol lattice (in Fourier space). In Fourier space it is then possible to carry out the z-summation analytically, leaving an absolutely convergent double sum in recipricol space (with the assumption of a slab-shaped form).

A distinction is made between the cases where the evaluation point does or does not lie in an x-y plane of dipoles ($\underline{z} = c\underline{a}_3$ or $z \neq c\underline{a}_3$, c an integer). In the first case the function to be summed has a simple pole (with respect to the z-summation) at $z = 0$. In this event an

auxilliary convergence function is used and the sum is broken up into two sums, one in real space over the x-y plane containing the evaluation point and one in recipricol space over the rest of the lattice. In the second case the function is everywhere regular and is Fourier transformed as it stands.

In either event the method is directly applicable only to lattices in which all dipoles are of the same magnitude and orientation. To evaluate the field of a lattice containing more than one orientation and/or magnitude of dipoles it is necessary to divide the lattice into sublattices, each containing only one kind of dipole, evaluate the field for each sublattice, and combine the fields by superposition.

The summation procedure, applied to a sublattice, produces nine numbers S_{ij} : i,j = x,y,z ; where S_{ij} is the i-component of the electric field (in Coulombs) due to a lattice of unit dipoles (one electronic charge and length 1Å) oriented in the j-direction.

While program inputs are in terms of the normal crystallographic quantities (a_1, a_2, a_3, $\alpha, \beta, \gamma, \delta$) the calculations and outputs are in terms of a cartesian reference frame related to the crystal basis vectors as detailed in figures 1-3.

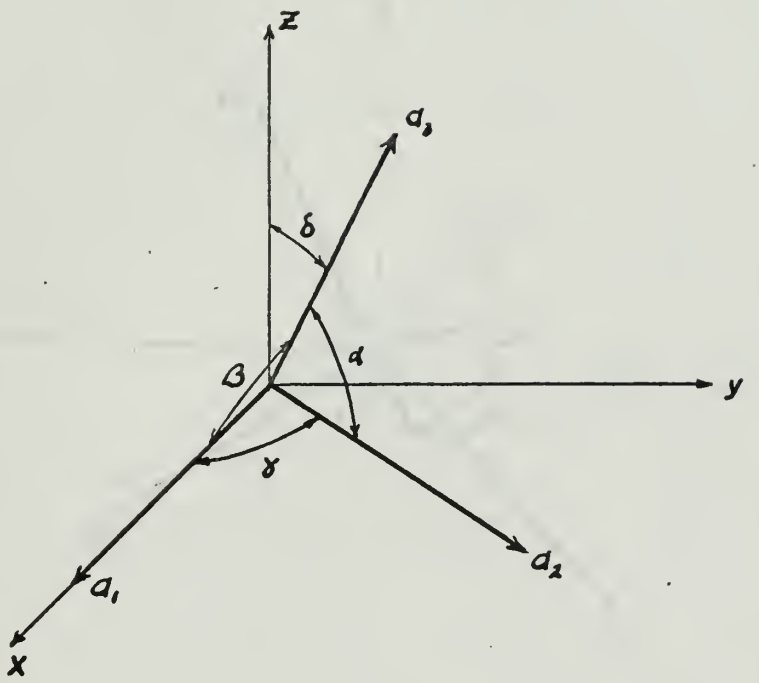


Figure 1: Unit Cell: 1 dipole per unit cell volume, Basis vectors $\underline{a}_1$, $\underline{a}_2$, $\underline{a}_3$. Crystal angles: $\alpha = \angle a_2, a_3$; $\beta = \angle a_1, a_3$; $\gamma = \angle a_1, a_2$; $\delta = \angle z, a_3$

x axis parallel to $\underline{a}_1$, y axis in $\underline{a}_1$ - $\underline{a}_2$ plane perpendicular to x axis, z axis perpendicular to x-y plane.

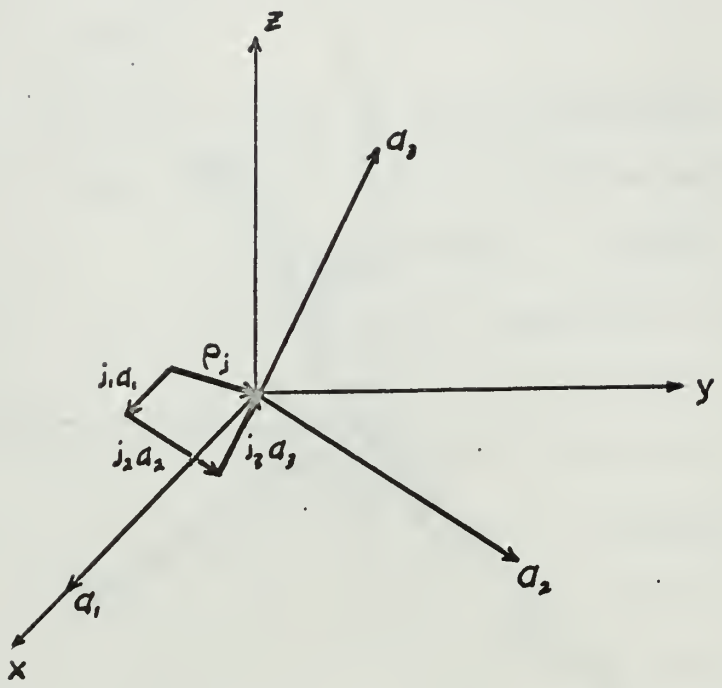


Figure 2: Point at which field is to be evaluated: located with respect to lattice point by fractions of basis vectors $\rho_j = j_1 a_1 + j_2 a_2 + j_3 a_3 \; ; \; 0 \leq j_i < 1$

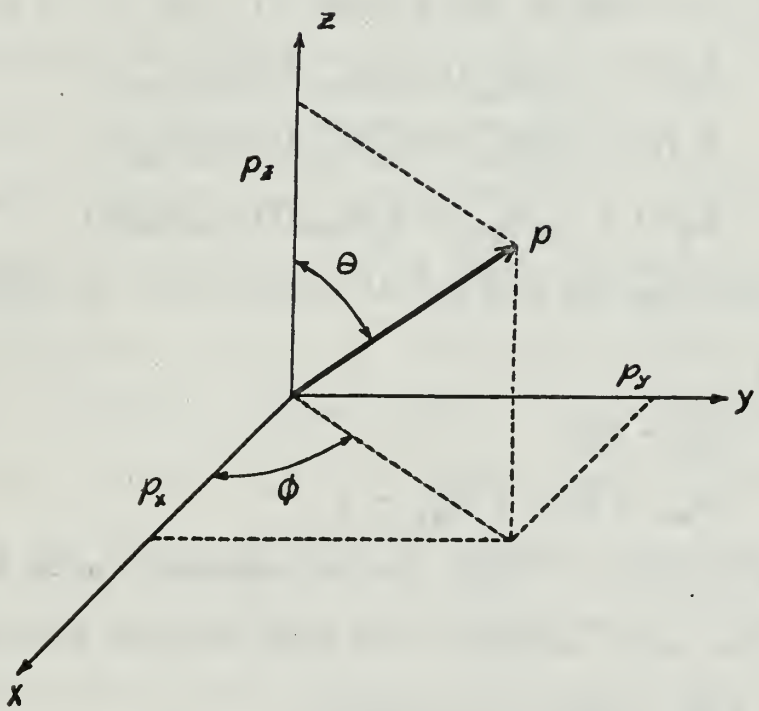


Figure 3: Decomposition of arbitrary dipole:

$$\underline{p} = p_x \hat{\imath} + p_y \hat{\jmath} + p_z \hat{k}$$

Then given a lattice of arbitrary dipoles $\underline{p}$, as in figure 3, we have:

$$p_x = p \sin\theta \cos\phi$$

$$p_y = p \sin\theta \sin\phi$$

$$p_z = p \cos\theta$$

so that the field at some point $j(j_1, j_2, j_3)$ is given by:

$$E_x(j) = p_x S_{xx}(j) + p_y S_{xy}(j) + p_z S_{xz}(j)$$

$$E_y(j) = p_x S_{yx}(j) + p_y S_{yy}(j) + p_z S_{yz}(j)$$

$$E_z(j) = p_x S_{zx}(j) + p_y S_{zy}(j) + p_z S_{zz}(j)$$

The nine S_{ij} are not all independent of course. They satisfy

$$S_{ij} = S_{ji}$$

$$S_{xx} + S_{yy} + S_{zz} = 0$$

for all lattices. Other special relations (such as $S_{ij} = 0$, $i \neq j$, for cubic lattices) are also obtained for lattices with a high order of symmetry.

In a lattice containing more than one kind of dipole two special considerations arise in decomposing the lattice into sublattices. First and most obviously, one must choose the j's in each sublattice, determining the point at which the fields are to be evaluated, such that they refer to a common point in the composite lattice. The second consideration refers back to the shape dependence of the

sum. In computing the sums over each sublattice, the shape dependence has introduced a depolarization factor $L = 4\pi/(\text{vol of unit cell in } \mathring{A}^3)$ into the S_{zz} sum. Then to superpose the fields from several sublattices with various z-directions (referred to the composite lattice) it is necessary to modify all the S_{ij} to bring all sublattices to a common x-y-z orientation by manipulating the depolarization factors for each sublattice. A similar consideration arises in comparing fields obtained by this method and those obtained by some other method which assumes a different crystal shape or with experimental results on a specific crystal of known shape. Kittel[5] considers the general problem of depolarization factors in some detail and tabulates the depolarization factors for most commonly used shapes (spherical, cubic, slab, etc.) An example of such considerations for a benzene model is contained in Appendix D.

[5]C. Kittel, Introduction to Solid State Physics, 2nd edition, 158, (John Wiley and Sons, Inc., New York, 1956)

PROGRAM COMPOSITION[6]

The actual translation of the method of Schacher and de Wette is relatively straightforward although quite lengthy.

The program is written in the FORTRAN 60 language for the CDC 1604 computer and is compatable with most FORTRAN monitors. The program is divided into a main program, containing all input-output routines and a segment to choose a subroutine, and eight subroutines to do the actual summation.

Simplified flow charts of the entire program and various segments are shown in figures 4-7.

[6] Appendix A contains the program listing and details of timing, storage, etc.

Figure 4: Flow Main Program - LATSUM

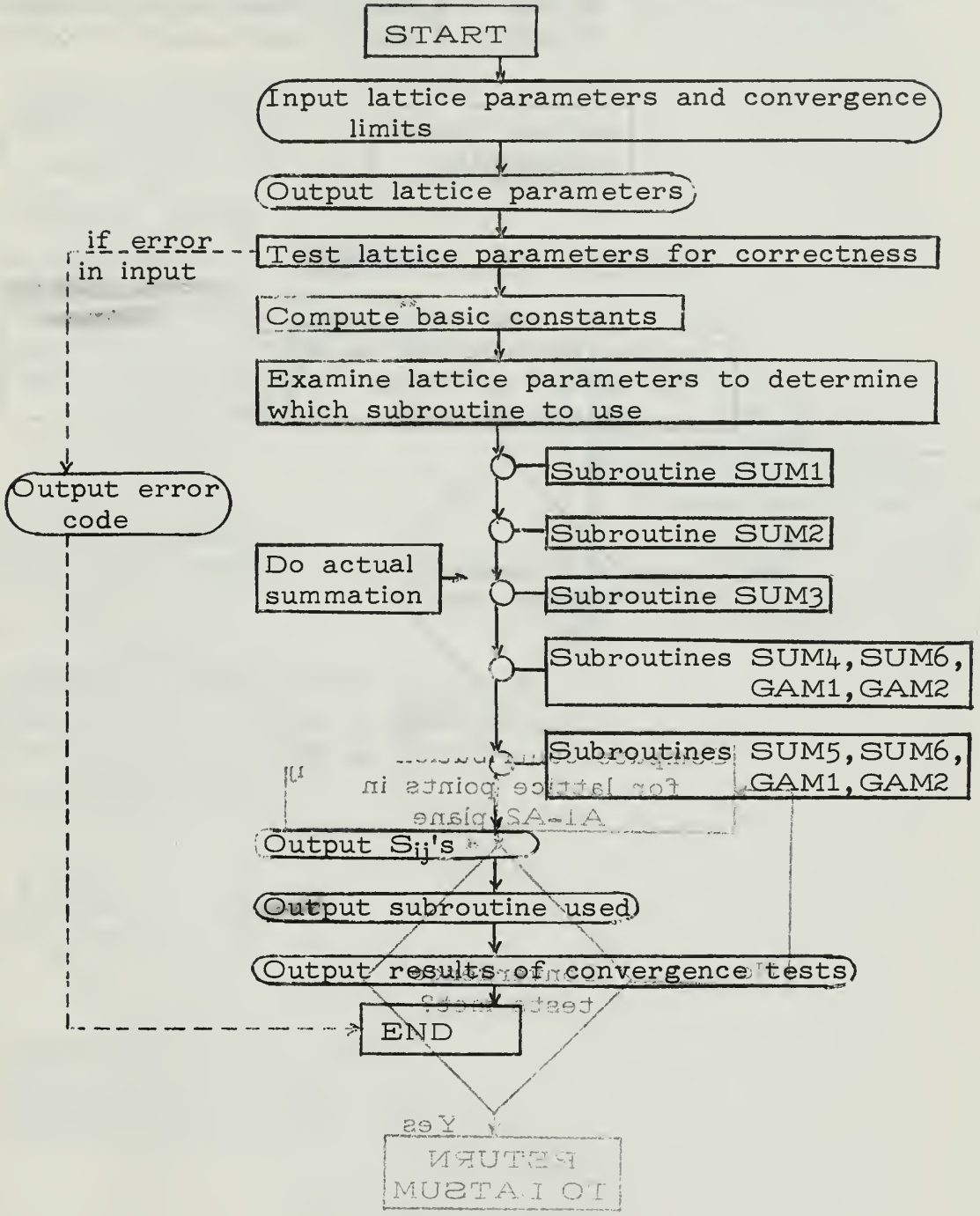


Figure 5: Common Flow-Subroutine SUM1, SUM2, SUM3

Main program uses SUM1 if XJ3≠0, XDEL≠0
SUM2 XJ3≠0, XDEL=0, XJ1+XJ2≠0
SUM3 XJ3≠0, XDEL=0, XJ1+XJ2=0

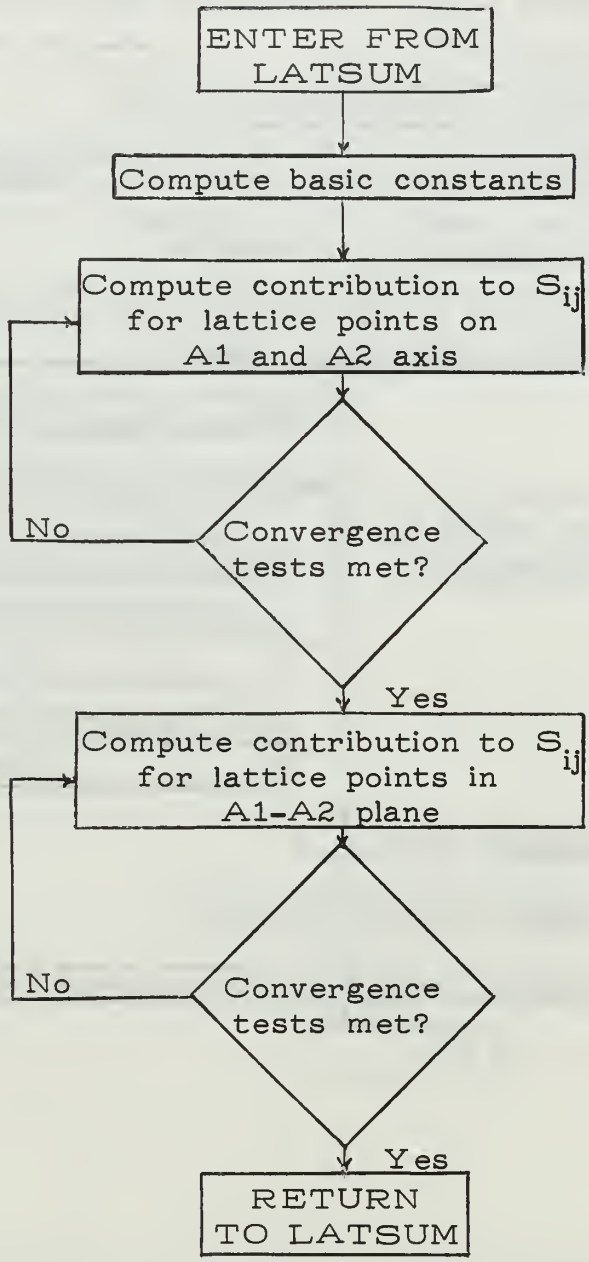


Figure 6: Common Flow - Subroutine SUM4, SUM5, GAM1

Main program uses SUM4 & SUM6 if XJ3=0, XDEL≠0
SUM5 & SUM6 if XJ3=0, XDEL=0

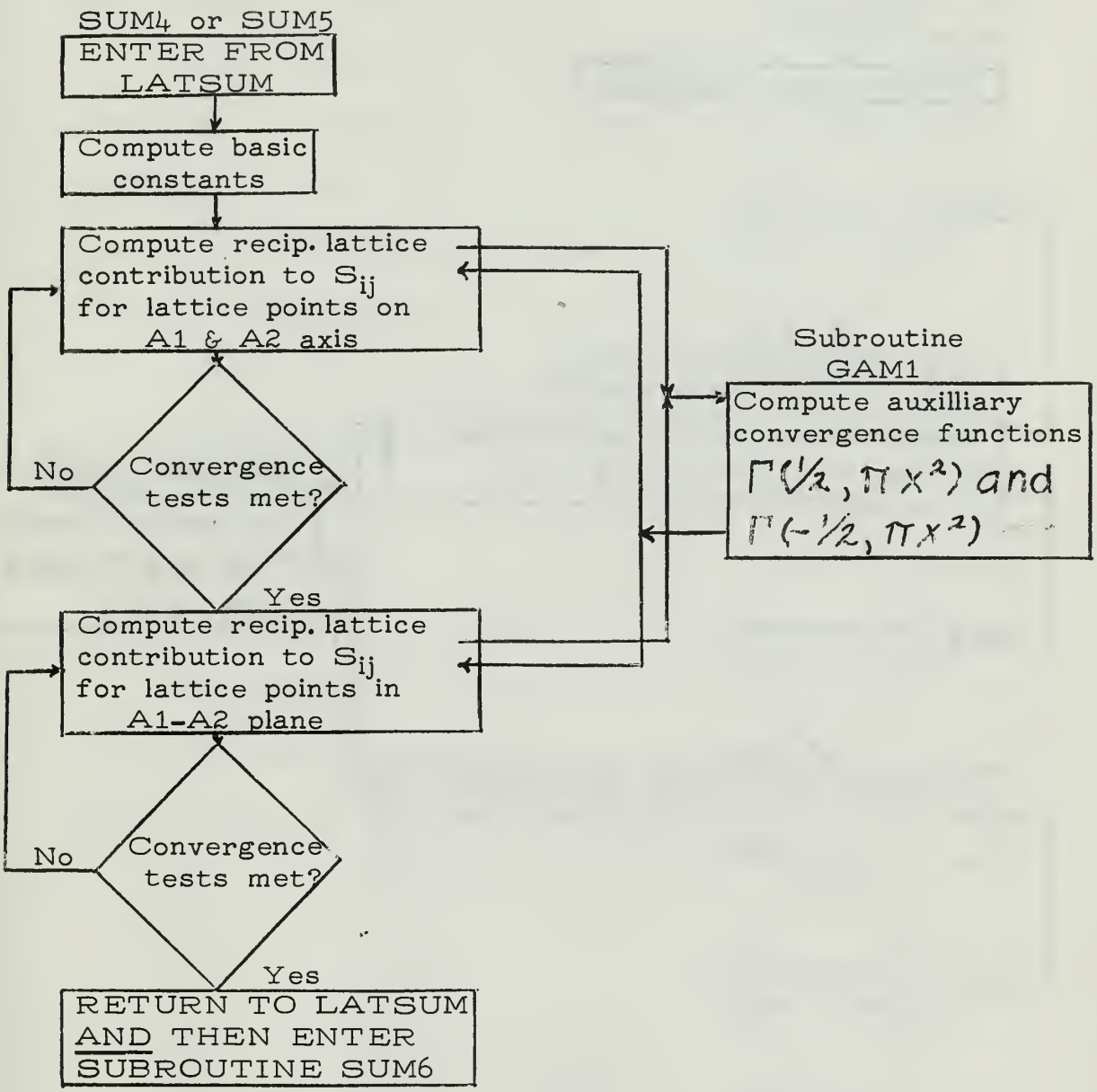
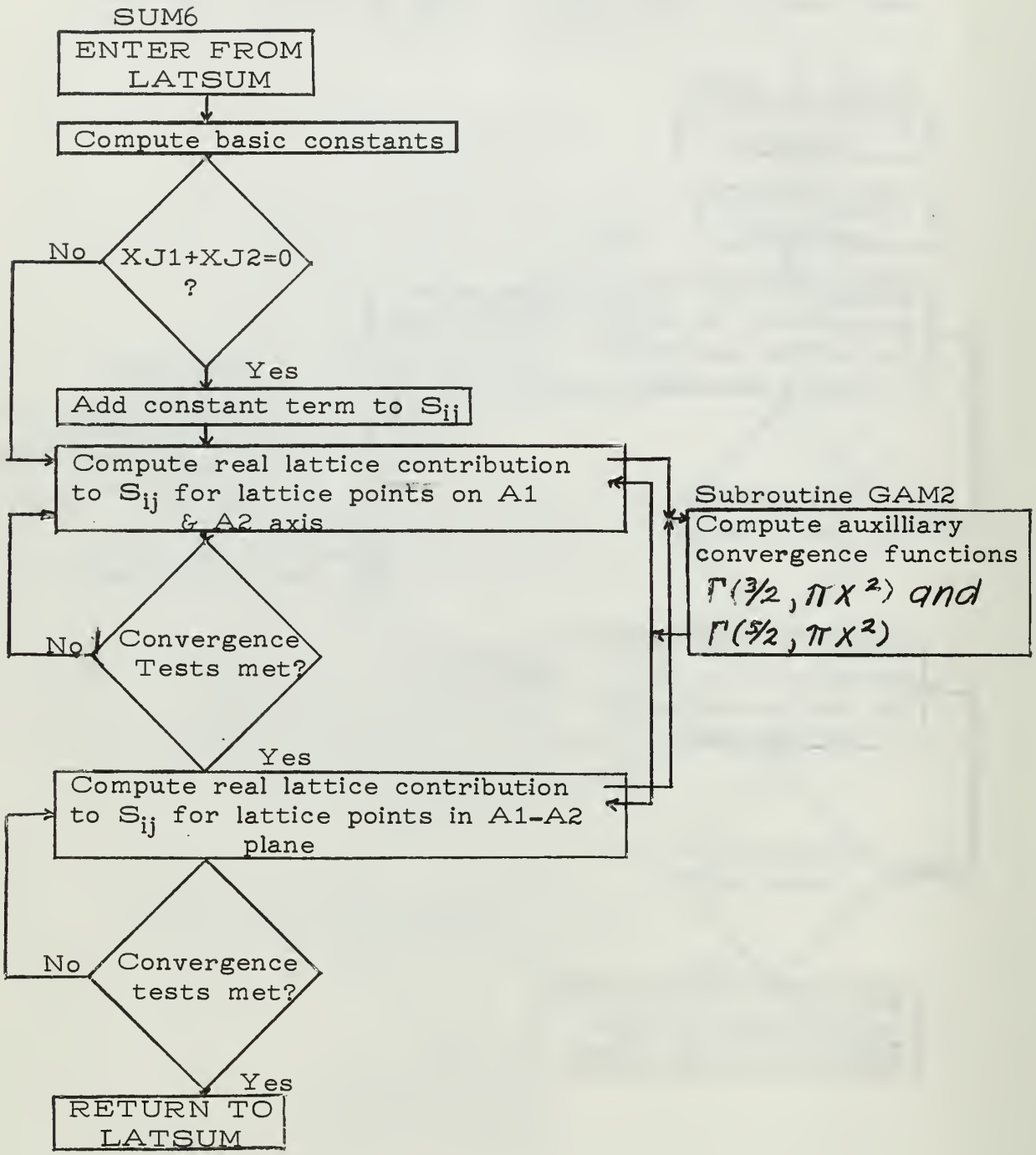


Figure 7: Flow Subroutine SUM6, GAM2

Used whenever XJ3=0



As can be seen from the flow charts, a deck can be made up for a particular lattice sum by appending to the main program either subroutines SUM1, SUM2, and SUM3 or subroutines SUM4, SUM5, SUM6, GAM1 and GAM2 depending on whether j_3 is not zero or zero respectively. Further, if sums are to be computed for several sets of data the main program deck can be modified by looping from the input segment to the END card.

Inputs to the program are given in Table 1.

Output is scattered throughout the main program. A check output of the input parameters always appears. If there is an error in the input parameters the following is printed and control returned to the monitor:

PROGRAM STOPPED BY INPUT ERROR

DESIGNATED BY K= _ _ _ _ _ _ _ _ _ _

The individual error codes are:

K	ERROR
1	A1 $\leq$ 0.
2	A2 $\leq$ 0.
4	A3 $\leq$ 0.
10	XJ1 $<$ 0. or XJ1 $>$ 1.
20	XJ2 $<$ 0. or XJ2 $>$ 1.
40	XJ3 $<$ 0. or XJ3 $>$ 1.
100	XALPH $\leq$ 0. or XALPH $>$ 90.
200	XBET $\leq$ 0. or XBET $>$ 90.
400	XGAM $\leq$ 0. or XGAM $\geq$ 180.
1000	XDEL $<$ 0. or XDEL $>$ 90.
2000	N $\leq$ 0

Table 1: Program Inputs

LABEL	UNITS	DESCRIPTION	ALLOWED LIMITS
A1 A2 A3	A	Length of basis vector a_i	$a_i > 0$
XJ1 XJ2 XJ3	Dimen sion less	j_i locating pt at which field is to be evaluated in terms of a_i (see figure 2)	$0 \leq j_i \leq 1$
XALPH XBET XGAM	Degrees and decimals	Crystal angles (see fig 1)	$0 < XALPH \leq 90$ $0 < XBET \leq 90$ $0 < XGAM < 180$
XDEL	degrees and decimals	Inclination of A3 axis from perpendicular .(see figure 1) Enter value if known else enter XDEL=90 and program will compute	$0 \leq XDEL \leq 90$
AEX REX AEY REY AEZ REZ	A⇒Å^{-1} R⇒ dimen sion less	Error limits for convergence tests. Summation will continue until the next term to be summed is less than $AE(y)^{(x)}+RE(y)^{(x)}$ times absolute $(z)\quad(z)$ value of sum at that time AEX&REX control S_{ix}&S_{xi} AEY&REY control S_{iy}&S_{yi} AEZ&REZ control S_{iz}&S_{zi} A fuller discussion is given in Appendix B	NONE
N	dimen sion less	Summation cutoff. Stops summation after covering 2N by 2N terms in x-y plane if convergence tests not met before then.	N > 0

Multiple errors result in a K value which is the sum of the individual K-values involved.

A second error output (and transfer back of control) occurs if N is so small that it is impossible to check the sums for convergence. This subject is covered more completely in appendix B. The printout is self-explanatory:

PROGRAM STOPPED BECAUSE N TOO SMALL.
N MUST BE AT LEAST - - + 1 TO ENSURE A GOOD TEST FOR CONVERGENCE.

These are the only error outputs contained in the program other than those that might arise from library routines. There are no error stops, pauses, dumps, sense switches or sense lights used.

Normal output (presuming no input errors) includes the nine sums S_{ij}, displayed as a labeled array. Following this is one of the statements:

SUMMING WAS DONE BY SUBROUTINE (SUM1) (SUM2) (SUM3)

WHICH ASSUMES (DELTA AND J3 BOTH DIFFERENT FROM ZERO)
(DELTA=0 BUT J1+J2 AND J3 NOT EQUAL TO ZERO)
(J1, J2, AND DELTA ALL ZERO BUT J3 NOT ZERO)

or

(SUM4 & SUM6)
SUMMING WAS DONE BY SUBROUTINES (SUM4 & SUM6)
(SUM5 & SUM6)
(SUM5 & SUM6)

(J3 = 0 BUT DELTA AND J1+J2 NOT ZERO)
ASSUMING (J1,J2, & J3 ALL ZERO BUT DELTA NOT ZERO)
(J3 AND DELTA ZERO BUT J1+J2 NOT ZERO)
(J1, J2, J3 AND DELTA ALL ZERO)

Following this is a statement of whether or not covergence test were met, and if not, a measure of the error introduced.

APPENDIX A

PROGRAM LISTING

A. IDENTIFICATION

Title	Electric Field Components by de Wette - Schacher Equations
Co-op Id.	Z1-NPGS-LATSUM (F-60,63)
Category	All Others
Programmer	David Dickmann
Date	February 1966

B. PURPOSE

This Fortram program computes electric fields per unit-dipoles for a lattice of similar dipoles. The program accepts lattices of any symmetry including triclinic and all higher symmetries, and computes field components in a cartesian reference frame, using the de Wette-Schacher equations.

C. USAGE

1. Calling sequence: This is a main program. See input formats.

2. Input arguments:

   A1, A2, A3 are the lengths, in Angstroms, of the lattice unit cell basis vectors.

   XJ1, XJ2, XJ3 are fractions of the basis vectors A1, A2, A3 designating the location of the point at which the fields are to be evaluated.

   XALPH is the crystal angle between the A2 and A3 axes, in degrees and decimals.

   XBET is the crystal angle between the A1 and A3 axes, in degrees and decimals.

   XGAM is the crystal angle between the A1 and A2 axes, in degrees and decimals.

XDEL is the inclination of the A3 axis from the perpendicular to the A1-A2 plane, in degrees and decimals. If unknown, enter as XDEL=90 and correct value is generated by program.

AEX, AEY, AEZ are the absolute error limits for the values of the x, y, and z components of the electric fields.

REX, REY, REZ are the relative error limits for the corresponding electric field components.

N is a summation cutoff value. If error limits are not met after $\sim 4N^2$ terms are summed, the program returns the field values at that time and a measure of the maximum error introduced by cutoff.

3. Space required: 6446 cells (F-60), 4209 cells (F-63)

4. Temporary storage: None

5. Alarms: None

6. Error returns:

   a. Error in input parameters--Control returned to monitor with printout:

      PROGRAM STOPPED BY INPUT

      ERROR DESIGNATED BY K= _ _

      Individual error codes are:

K	Error
1	A1 $\leq$ 0.
2	A2 $\leq$ 0.
4	A3 $\leq$ 0.
10	XJ1 $<$ 0. or XJ1 $>$ 1.
20	XJ2 $<$ 0. or XJ2 $>$ 1.
40	XJ3 $<$ 0. or XJ3 $>$ 1.
100	XALPH $\leq$ 0. or XALPH $>$ 90.
200	XBET $\leq$ 0. or XBET $>$ 90.

400 XGAM $\leq$ 0. or XGAM $\geq$ 180.
1000 XDEL $<$ 0. or XDEL $>$ 90.
2000 N $\leq$ 0

Multiple errors result in a K value which is the sum of the individual values above.

b. N value too small to ensure good test for convergence of field sums. Control returned to monitor with self-explanatory printout.

7. Error Stops: None except those associated with machine arithmetic errors.

8. Input and output tape mountings: Normal

9. Input and output formats

a. Input is contained on four cards under the following format control:

```
READ 1,A1,A2,A3,XJ1,XJ2,XJ3,XALPH,
     XBET,XGAM,XDEL,N,AEX,REX,
     AEY,REY,AEZ,REZ
1 FORMAT (3F10.0/3F10.0/4F10.0/I4,6E10.0)
```

b. Output: Various

(1) Error outputs as per 6

(2) S_{ij} - - the i-th component of the electric field due to a unit dipole oriented in the j-direction. Printed as an array under 1PE19.10 with labels SUMXX, etc.

(3) Hollerith prints indicating subroutines used and results of convergence tests.

10. Selective stop and jump settings: Not applicable

11. Timing:

a. Compile time: 4 min 20 sec

b. Run time: Average 1.4 sec per lattice, averaged over 336 combinations of lattices, error limits, and evaluation points.

12. Accuracy: Relative error of $S_{ij} \leq \min_{i,j}(REX, REY, REZ) * S_{ij}$
Absolute error of $S_{ij} \leq \min_{i,j}(AEX, AEY, AEZ)$

13. Equipment configuration: CDC 1604 with FORTRAN compiler or CO-OP monitor system including F-63

14. Library routines used:
SQRTF
SINF
COSF
ATANF
ASINF
ACOSF
EXPF
ABSF
FIXFLOAT
FLOAT FIX

15. References:

a. D. B. DICKMANN, A Computer Program for Evaluating Lattice Sums, Thesis, U.S. Naval Postgraduate School, Monterey, 1966

b. F. W. de Wette and G. E. Schacher, Phys. Rev., 137, A78 (1965)

D. METHOD OF ALGORITHM See references (a) and (b).

E. FLOW CHART See reference (a).

```
      PROGRAM LATSUM                                                    MN0001
     0COMMON A1,A2,A3,XJ1,XJ2,XJ3,XALPH,XBET,XGAM,XDEL,AEX,REX,AEY,REY,A MN0002
     1EZ,REZ,AEXY,REXY,AEXZ,REXZ,AEYZ,REYZ,L,M,N,LL,MM,LINE1,LINE2,NILE1 MN0003
     2,NILE2,MIRE,BIGO,BIG,CIGO,CIG,RTMXX,RTMXY,RTMXZ,RTMYY,RTMYZ,RTMZZ, MN0004
     3RSUMXX,RSUMXY,RSUMXZ,RSUMYY,RSUMYZ,RSUMZZ,SUMXX,SUMXY,SUMXZ,SUMYY, MN0005
     4SUMYZ,SUMZZ,PI,SPI,SIGAM,CTGAM,COGAM,COALPH,COBET,CODEL,SIDEL,OA,V MN0006
     5OL,POW,POW3,PV1,PV2,TE,CS1,CS2,AMP,JIG,XSI1,XSI2,ADD,RATIO,XMU1,XM MN0007
     6U2,S1,S2,SV1,SV2,SV3,H1,H2,HX1,HX2,HY1,HY2,W1,W2,Z1,Z2,X11,X12,X21 MN0008
     7,X22,Y11,Y12,Y21,Y22,ROMG31,ROMG32,COMG31,COMG32,GP11,GP12,GM11,GM MN0009
     812,GP31,GP32,GP51,GP52,T11,T12,T21,T22,T31,T32,T41,T42,T51,T52,T61 MN0010
     9,T62,T71,T72,T81,T82                                              MN0011
      DIMENSION C(17)                                                   MN0012
      COMMON C                                                          MN0013
     OREAD 1,A1,A2,A3,XJ1,XJ2,XJ3,XALPH,XBET,XGAM,XDEL,N,AEX,REX,AEY,REY MN0014
     1,AEZ,REZ                                                          MN0015
    1 FORMAT (3F10.0/3F10.0/4F10.0/I4,6E10.0)                           MN0016
      PRINT 21                                                          MN0017
   21 FORMAT (25H0     INPUT PARAMETERS - -)                            MN0018
      PRINT 22,A1,A2,A3                                                 MN0019
   22 FORMAT (13H0           A1=,F10.6,7H,    A2=,F10.6,7H,    A3=,F10.6) MN0020
      PRINT 23,XJ1,XJ2,XJ3                                              MN0021
   23 FORMAT (14H0          XJ1=,F10.6,7H,  XJ2=,F10.6,7H,  XJ3=,F10.6) MN0022
      PRINT 24,XALPH,XBET,XGAM,XDEL                                     MN0023
   24 FORMAT (16H0         XALPH=,F10.6,7H, XBET=,F10.6,7H, XGAM=,F10.6, MN0024
     17H, XDEL=,F10.6)                                                  MN0025
      PRINT 25,N,AEX,REX,AEY,REY,AEZ,REZ                                MN0026
   25 FORMAT (12H0           N=,I4,7H,  AEX=,1PE10.3,7H,  REX=,1PE10.3,7H, MN0027
     1  AEY=,1PE10.3,7H,  REY=,1PE10.3,7H,  AEZ=,1PE10.3,7H,  REZ=,1PE10 MN0028
     2.3)                                                               MN0029
      PRINT 26                                                          MN0030
   26 FORMAT (26H0     OUTPUT PARAMETERS - -)                           MN0031
      IF(AEX-AEY) 2,2,3                                                 MN0032
    2 AEXY=AEX                                                          MN0033
      GO TO 4                                                           MN0034
    3 AEXY=AEY                                                          MN0035
    4 IF(REX-REY) 5,5,6                                                 MN0036
    5 REXY=REX                                                          MN0037
      GO TO 7                                                           MN0038
    6 REXY=REY                                                          MN0039
    7 IF(AEX-AEZ) 8,8,9                                                 MN0040
    8 AEXZ=AEX                                                          MN0041
      GO TO 10                                                          MN0042
    9 AEXZ=AEZ                                                          MN0043
   10 IF(REX-REZ) 11,11,12                                              MN0044
   11 REXZ=REX                                                          MN0045
      GO TO 13                                                          MN0046
   12 REXZ=REZ                                                          MN0047
   13 IF(AEY-AEZ) 14,14,15                                              MN0048
```

```
14 AEYZ=AEY                                                          MN0049
   GO TO 16                                                          MN0050
15 AEYZ=AEZ                                                          MN0051
16 IF(REY-REZ) 17,17,18                                              MN0052
17 REYZ=REY                                                          MN0053
   GO TO 19                                                          MN0054
18 REYZ=REZ                                                          MN0055
19 K=0                                                               MN0056
   IF(A1) 30,30,31                                                   MN0057
30 K=K+1                                                             MN0058
31 IF(A2) 32,32,33                                                   MN0059
32 K=K+2                                                             MN0060
33 IF(A3) 34,34,35                                                   MN0061
34 K=K+4                                                             MN0062
35 IF(XJ1) 37,39,36                                                  MN0063
36 IF(XJ1-1.)39,38,37                                                MN0064
37 K=K+10                                                            MN0065
   GO TO 39                                                          MN0066
38 XJ1=0.                                                            MN0067
39 IF(XJ2) 41,43,40                                                  MN0068
40 IF(XJ2-1.) 43,42,41                                               MN0069
41 K=K+20                                                            MN0070
   GO TO 43                                                          MN0071
42 XJ2=0.                                                            MN0072
43 IF(XJ3) 45,47,44                                                  MN0073
44 IF(XJ3-1.)47,46,45                                                MN0074
45 K=K+40                                                            MN0075
   GO TO 20                                                          MN0076
46 XJ3=0.                                                            MN0077
47 L=0                                                               MN0078
20 IF(XALPH) 49,49,48                                                MN0079
48 IF(XALPH-90.) 51,50,49                                            MN0080
49 K=K+100                                                           MN0081
   GO TO 51                                                          MN0082
50 L=L+1                                                             MN0083
51 IF(XBET) 53,53,52                                                 MN0084
52 IF(XBET-90.) 55,54,53                                             MN0085
53 K=K+200                                                           MN0086
   GO TO 55                                                          MN0087
54 L=L+1                                                             MN0088
55 IF(XGAM) 57,57,56                                                 MN0089
56 IF(XGAM-180.) 58,57,57                                            MN0090
57 K=K+400                                                           MN0091
58 IF(XDEL) 60,61,59                                                 MN0092
59 IF(XDEL-90.) 61,61,60                                             MN0093
60 K=K+1000                                                          MN0094
61 IF(N) 62,62,63                                                    MN0095
62 K=K+2000                                                          MN0096
```

```
63 IF(K) 64,66,64                                                              MN0097
64 PRINT 65,K                                                                  MN0098
650FORMAT (61HO    PROGRAM STOPPED BECAUSE OF INPUT ERROR DESIGNATED           MN0099
  1BY K= ,I4)                                                                  MN0100
   GO TO 999                                                                   MN0101
66 PI=ATANF(1.)*4.                                                             MN0102
   CONV=PI/180.                                                                MN0103
   ALPH=XALPH*CONV                                                             MN0104
   BET=XBET*CONV                                                               MN0105
   GAM=XGAM*CONV                                                               MN0106
   COALPH=COSF(ALPH)                                                           MN0107
   COBET=COSF(BET)                                                             MN0108
   COGAM=COSF(GAM)                                                             MN0109
   SIGAM=SINF(GAM)                                                             MN0110
   CTGAM=COGAM/SIGAM                                                           MN0111
   RATIO=A3/A1                                                                 MN0112
   K=1                                                                         MN0113
   IF(XDEL) 83,83,81                                                           MN0114
81 IF(XDEL-90.) 84,82,82                                                       MN0115
82 IF(L-2) 85,83,83                                                            MN0116
83 DEL=0.                                                                      MN0117
   CODEL=1.                                                                    MN0118
   SIDEL=0.                                                                    MN0119
   XSI1=C.                                                                     MN0120
   XSI2=C.                                                                     MN0121
   K=K+1                                                                       MN0122
   GO TO 87                                                                    MN0123
84 DEL=XDEL*CONV                                                               MN0124
   GO TO 86                                                                    MN0125
850DEL=ASINF(SQRTF(COALPH*COALPH+COBET*COBET-2.*COGAM*COALPH*COBET)/S          MN0126
  1IGAM)                                                                       MN0127
86 CODEL=COSF(DEL)                                                             MN0128
   SIDEL=SINF(DEL)                                                             MN0129
   IF(COBET-SIDEL)68,67,67                                                     MN0130
67 T11=0.                                                                      MN0131
   GO TO 69                                                                    MN0132
68 T11=ACOSF(COBET/SIDEL)                                                      MN0133
   IF(COALPH-COBET*COGAM)70,69,69                                              MN0134
70 T11=-T11                                                                    MN0135
69 T12=SINF(T11)                                                               MN0136
   T21=RATIO*SIDEL                                                             MN0137
   XSI1=(-T12*CTGAM+CCSF(T11))*T21                                             MN0138
   T22=A3*SIDEL/A2                                                             MN0139
   XSI2=T22*T12/SIGAM                                                          MN0140
87 OA=A2*SIGAM/A1                                                              MN0141
   VOL=A1*A1*A1                                                                MN0142
   POW=-2.*PI*CODEL*RATIO                                                      MN0143
   POW3=-POW*XJ3                                                               MN0144
```

```
      PV1=(XJ3*XSI1+XJ1)*2.*PI                                                  MN0145
      PV2=(XJ3*XSI2+XJ2)*2.*PI                                                  MN0146
      TE=1./OA                                                                  MN0147
      CS1=2.*PI*XSI1                                                            MN0148
      CS2=2.*PI*XSI2                                                            MN0149
      AMP=4.*PI*PI*TE/VOL                                                       MN0150
      SPI=SQRTF(PI)                                                             MN0151
      C(1)=4.981466305480E-03                                                   MN0152
      C(2)=-4.603839021001E-02                                                  MN0153
      C(3)=1.962335473654E-01                                                   MN0154
      C(4)=-5.126090482518E-01                                                  MN0155
      C(5)=9.207978817867E-01                                                   MN0156
      C(6)=-1.212006515707                                                      MN0157
      C(7)=1.220575567626                                                       MN0158
      C(8)=-9.759727701312E-01                                                  MN0159
      C(9)=6.459040706104E-01                                                   MN0160
      C(10)=-3.745177000383E-01                                                 MN0161
      C(11)=2.063608822646E-01                                                  MN0162
      C(12)=-1.196819795259E-01                                                 MN0163
      C(13)=8.087599303690E-02                                                  MN0164
      C(14)=-6.943757087720E-02                                                 MN0165
      C(15)=8.333315543132E-02                                                  MN0166
      C(16)=-1.666666648161E-01                                                 MN0167
      C(17)=9.999999999709E-01                                                  MN0168
      IF(A1-A2) 88,88,89                                                        MN0169
   88 JIG=2.*A2*COGAM/A1+1.                                                     MN0170
      GO TO 90                                                                  MN0171
   89 JIG=2.*A1*COGAM/A2+1.                                                     MN0172
   90 IF(JIG-N)94,91,91                                                         MN0173
   91 PRINT 92,JIG                                                              MN0174
  920FORMAT (62HO    PROGRAM STOPPED BECAUSE N TOO SMALL.  N MUST BE AT MN0175
     1 LEAST ,I4, 15H + 1  TO ENSURE)                                           MN0176
      PRINT 93                                                                  MN0177
   93 FORMAT (33H      A GOOD TEST FOR CONVERGENCE.)                            MN0178
      GO TO 999                                                                 MN0179
   94 BIGO=C.                                                                   MN0180
      BIG=0.                                                                    MN0181
      L=0                                                                       MN0182
      M=0                                                                       MN0183
      LINE1=0                                                                   MN0184
      LINE2=0                                                                   MN0185
      CIGO=C.                                                                   MN0186
      CIG=0.                                                                    MN0187
      LL=0                                                                      MN0188
      MM=0                                                                      MN0189
      NILE1=0                                                                   MN0190
      NILE2=0                                                                   MN0191
      IF(XJ1+XJ2) 96,95,96                                                      MN0192
```

```
 95 K=K+2                                                              MN0193
 96 IF(XJ3) 98,97,98                                                   MN0194
 97 K=K+4                                                              MN0195
 98 RSUMXX=0.                                                          MN0196
    RSUMXY=0.                                                          MN0197
    RSUMXZ=0.                                                          MN0198
    RSUMYY=0.                                                          MN0199
    RSUMYZ=0.                                                          MN0200
    RSUMZZ=0.                                                          MN0201
    SUMXX=0.                                                           MN0202
    SUMXY=0.                                                           MN0203
    SUMXZ=0.                                                           MN0204
    SUMYY=0.                                                           MN0205
    SUMYZ=0.                                                           MN0206
    SUMZZ=0.                                                           MN0207
    T11=1./AMP                                                         MN0208
    AEX=AEX*T11                                                        MN0209
    REX=REX*T11                                                        MN0210
    AEY=AEY*T11                                                        MN0211
    REY=REY*T11                                                        MN0212
    AEZ=AEZ*T11                                                        MN0213
    REZ=REZ*T11                                                        MN0214
    AEXY=AEXY*T11                                                      MN0215
    REXY=REXY*T11                                                      MN0216
    AEXZ=AEXZ*T11                                                      MN0217
    REXZ=REXZ*T11                                                      MN0218
    AEYZ=AEYZ*T11                                                      MN0219
    REYZ=REYZ*T11                                                      MN0220
    GO TO (101,102,101,103,105,107,105,107),K                          MN0221
101 CALL SUM1                                                          MN0222
    GO TO 108                                                          MN0223
102 CALL SUM2                                                          MN0224
    GO TO 108                                                          MN0225
103 CALL SUM3                                                          MN0226
    GO TO 108                                                          MN0227
105 CALL SUM4                                                          MN0228
    CALL SUM6                                                          MN0229
    GO TO 108                                                          MN0230
107 CALL SUM5                                                          MN0231
    CALL SUM6                                                          MN0232
108 SUMYX=SUMXY                                                        MN0233
    SUMZX=SUMXZ                                                        MN0234
    SUMZY=SUMYZ                                                        MN0235
    T11=AMP                                                            MN0236
    AEX=AEX*T11                                                        MN0237
    REX=REX*T11                                                        MN0238
    AEY=AEY*T11                                                        MN0239
    REY=REY*T11                                                        MN0240
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      AEZ=AEZ*T11                                                       MN0241
      REZ=REZ*T11                                                       MN0242
      AEXY=AEXY*T11                                                     MN0243
      REXY=REXY*T11                                                     MN0244
      AEXZ=AEXZ*T11                                                     MN0245
      REXZ=REXZ*T11                                                     MN0246
      AEYZ=AEYZ*T11                                                     MN0247
      REYZ=REYZ*T11                                                     MN0248
      PRINT 109,SUMXX,SUMXY,SUMXZ                                       MN0249
  109 FORMAT (11HO    SUMXX=,1PE19.10,11H     SUMXY=,1PE19.10,11H     SU MN0250
     1MXZ=,1PE19.10)                                                    MN0251
      PRINT 110,SUMYX,SUMYY,SUMYZ                                       MN0252
  110 FORMAT (11HO    SUMYX=,1PE19.10,11H     SUMYY=,1PE19.10,11H     SU MN0253
     1MYZ=,1PE19.10)                                                    MN0254
      PRINT 111,SUMZX,SUMZY,SUMZZ                                       MN0255
  111 FORMAT (11HO    SUMZX=,1PE19.10,11H     SUMZY=,1PE19.10,11H     SU MN0256
     1MZZ=,1PE19.10)                                                    MN0257
      GO TO (126,128,130,132,134,137,139),MIRE                          MN0258
  126 PRINT 127                                                         MN0259
 1270FORMAT (92HO    SUMMING WAS DONE BY SUBROUTINE SUM1 WHICH ASSUMES  MN0260
     1DELTA AND J3 BOTH DIFFERENT FROM ZERO)                            MN0261
      GO TO 136                                                         MN0262
  128 PRINT 129                                                         MN0263
 1290FORMAT (97HO    SUMMING WAS DONE BY SUBROUTINE SUM2 WHICH ASSUMES  MN0264
     1DELTA=0 BUT J1+J2 AND J3 NOT EQUAL TO ZERO)                       MN0265
      GO TO 136                                                         MN0266
  130 PRINT 131                                                         MN0267
 1310FORMAT (95HO    SUMMING WAS DONE BY SUBROUTINE SUM3 WHICH ASSUMES  MN0268
     1J1,J2,AND DELTA ALL ZERO BUT J3 NOT ZERO)                         MN0269
      GO TO 136                                                         MN0270
  132 PRINT 133                                                         MN0271
  133 FORMAT (94HO    SUMMING WAS DONE BY SUBROUTINES SUM4 AND SUM6, ASS MN0272
     1UMING J3=0 BUT DELTA AND J1+J2 NOT ZERO)                          MN0273
      GO TO 136                                                         MN0274
  134 PRINT 135                                                         MN0275
  135 FORMAT(102HO    SUMMING WAS DONE BY SUBROUTINES SUM4 AND SUM6, ASS MN0276
     1UMING J1,J2, AND J3 ALL ZERO BUT DELTA NOT ZERO)                  MN0277
      GO TO 136                                                         MN0278
  137 PRINT 138                                                         MN0279
  138 FORMAT (97HO    SUMMING WAS DONE BY SUBROUTINES SUM5 AND SUM6, ASS MN0280
     1UMING J3 AND DELTA ZERO BUT J1+J2 NOT ZERO)                       MN0281
      GO TO 136                                                         MN0282
  139 PRINT 140                                                         MN0283
  140 FORMAT (91HO    SUMMING WAS DONE BY SUBROUTINES SUM5 AND SUM6, ASS MN0284
     1UMING J1, J2, J3, AND DELTA ALL ZERO)                             MN0285
  136 PRINT 141                                                         MN0286
  141 FORMAT (39HO    FOR THE RECIPRICOL LATTICE SUM - -)               MN0287
      IF(BIGO)114,112,114                                               MN0288
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112 PRINT 113                                                          MN0289
113 FORMAT (52HO    CONVERGENCE TESTS WERE MET FOR THE AXIAL TERMS.)   MN0290
    GO TO 116                                                          MN0291
114 PRINT 115,BIGO                                                     MN0292
1150FORMAT (86HO    CONVERGENCE TESTS WERE NOT MET FOR THE AXIAL TERMS MN0293
   1.  THE LARGEST TERM DROPPED WAS,1PE16.7)                           MN0294
116 IF(L+M) 117,117,119                                                MN0295
117 PRINT 118                                                          MN0296
118 FORMAT (52HO    CONVERGENCE TESTS WERE MET FOR OFF-AXIAL TERMS.)   MN0297
    GO TO 142                                                          MN0298
119 IF(M)123,123,121                                                   MN0299
121 PRINT 122                                                          MN0300
1220FORMAT (84HO    N WAS TOO SMALL TO ENSURE CONVERGENCE OF OFF-AXIAL MN0301
   1 TERMS FOR LARGER VALUES OF X)                                     MN0302
    IF(L)142,142,123                                                   MN0303
123 PRINT 124,L,LINE1                                                  MN0304
1240FORMAT (56HO    CONVERGENCE TESTS WERE NOT MET FOR OFF-AXIAL TERMS MN0305
   1.,I6,23H VALUES OF X BETWEEN X=,I6,4H AND)                         MN0306
    PRINT 125,LINE2,BIG                                                MN0307
1250FORMAT (7H      X=,I6,57H GAVE EXCESSIVE TERMS FOR Y=N.  THE LARGES MN0308
   1T SUCH TERM WAS,1PE16.7)                                           MN0309
142 IF(MIRE-3)143,143,145                                              MN0310
143 PRINT 144                                                          MN0311
144 FORMAT (62HO    REAL LATTICE SUMS WERE NOT REQUIRED SINCE J3 WAS N MN0312
   1OT ZERO)                                                           MN0313
    GO TO 999                                                          MN0314
145 PRINT 146                                                          MN0315
146 FORMAT (33HO    FOR THE REAL LATTICE SUM - -)                      MN0316
    IF(CIGO)148,147,148                                                MN0317
147 PRINT 113                                                          MN0318
    GO TO 149                                                          MN0319
148 PRINT 115,CIGO                                                     MN0320
149 IF(LL+MM)150,150,151                                               MN0321
150 PRINT 118                                                          MN0322
    GO TO 999                                                          MN0323
151 IF(MM)153,153,152                                                  MN0324
152 PRINT 122                                                          MN0325
    IF(LL)999,999,153                                                  MN0326
153 PRINT 124,LL,NILE1                                                 MN0327
    PRINT 125,NILE2,CIG                                                MN0328
999 STOP                                                               MN0329
    END                                                                MN0330
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 SUBROUTINE SUM1                                                                 1S0000
0COMMON A1,A2,A3,XJ1,XJ2,XJ3,XALPH,XBET,XGAM,XDEL,AEX,REX,AEY,REY,A              1S0001
1EZ,REZ,AEXY,REXY,AEXZ,REXZ,AEYZ,REYZ,L,M,N,LL,MM,LINE1,LINE2,NILE1             1S0002
2,NILE2,MIRE,BIGO,BIG,CIGO,CIG,RTMXX,RTMXY,RTMXZ,RTMYY,RTMYZ,RTMZZ,             1S0003
3RSUMXX,RSUMXY,RSUMXZ,RSUMYY,RSUMYZ,RSUMZZ,SUMXX,SUMXY,SUMXZ,SUMYY,             1S0004
4SUMYZ,SUMZZ,PI,SPI,SIGAM,CTGAM,COGAM,COALPH,COBET,CODEL,SIDEL,CA,V              1S0005
5OL,POW,POW3,PV1,PV2,TE,CS1,CS2,AMP,JIG,XSI1,XSI2,ADD,RATIC,XMU1,XM              1S0006
6U2,S1,S2,SV1,SV2,SV3,H1,H2,HX1,HX2,HY1,HY2,W1,W2,Z1,Z2,X11,X12,X21              1S0007
7,X22,Y11,Y12,Y21,Y22,ROMG31,ROMG32,COMG31,COMG32,GP11,GP12,GM11,GM              1S0008
812,GP31,GP32,GP51,GP52,T11,T12,T21,T22,T31,T32,T41,T42,T51,T52,T61              1S0009
9,T62,T71,T72,T81,T82                                                           1S0010
 MIRE=1                                                                         1S0011
 DO 6 I=1,N                                                                     1S0012
 XMU1=I                                                                         1S0013
 H1=XMU1/SIGAM                                                                  1S0014
 T11=PV1*XMU1                                                                   1S0015
 X11=CCSF(T11)                                                                  1S0016
 X21=SINF(T11)                                                                  1S0017
 T11=CS1*XMU1                                                                   1S0018
 Y11=CCSF(T11)                                                                  1S0019
 Y21=SINF(T11)                                                                  1S0020
 W1=EXPF(POW*H1)                                                                1S0021
 Z1=EXPF(POW3*H1)                                                               1S0022
 T11=1./Z1                                                                      1S0023
 T21=1./W1                                                                      1S0024
 T31=X11*Y11+X21*Y21                                                            1S0025
 T41=X21*Y11-X11*Y21                                                            1S0026
 T51=-2.*Y11+T21+W1                                                             1S0027
 T61=W1*Z1                                                                      1S0028
 T71=T11*T21                                                                    1S0029
 T81=1./T51                                                                     1S0030
 ROMG31=((Z1-T11)*T31-(T61-T71)*X11)*T81                                        1S0031
 COMG31=((Z1+T11)*T41-(T61+T71)*X21)*T81                                        1S0032
 RTMXX=-2.*XMU1*SIGAM*ROMG31                                                    1S0033
 RTMXY=-RTMXX*CTGAM                                                             1S0034
 RTMXZ=-2.*XMU1*COMG31                                                          1S0035
 RTMYY=CTGAM*CTGAM*RTMXX                                                        1S0036
 RTMYZ=-CTGAM*RTMXZ                                                             1S0037
 RTMZZ=2.*H1*ROMG31                                                             1S0038
 XMU2=XMU1                                                                      1S0039
 H1=XMU2*TE                                                                     1S0040
 T11=PV2*XMU2                                                                   1S0041
 X11=CCSF(T11)                                                                  1S0042
 X21=SINF(T11)                                                                  1S0043
 T11=CS2*XMU2                                                                   1S0044
 Y11=CCSF(T11)                                                                  1S0045
 Y21=SINF(T11)                                                                  1S0046
 W1=EXPF(POW*H1)                                                                1S0047
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      Z1=EXPF(POW3*H1)                                                  1S0048
      T11=1./Z1                                                         1S0049
      T21=1./W1                                                         1S0050
      T31=X11*Y11+X21*Y21                                               1S0051
      T41=X21*Y11-X11*Y21                                               1S0052
      T51=-2.*Y11+T21+W1                                                1S0053
      T61=W1*Z1                                                         1S0054
      T71=T11*T21                                                       1S0055
      T81=1./T51                                                        1S0056
      ROMG31=((Z1-T11)*T31-(T61-T71)*X11)*T81                           1S0057
      COMG31=((Z1+T11)*T41-(T61+T71)*X21)*T81                           1S0058
      RTMYY=RTMYY-2.*H1*ROMG31                                          1S0059
      RTMYZ=RTMYZ-2.*H1*COMG31                                          1S0060
      RTMZZ=RTMZZ+2.*H1*ROMG31                                          1S0061
      RSUMXX=RSUMXX+RTMXX                                               1S0062
      RSUMXY=RSUMXY+RTMXY                                               1S0063
      RSUMXZ=RSUMXZ+RTMXZ                                               1S0064
      RSUMYY=RSUMYY+RTMYY                                               1S0065
      RSUMYZ=RSUMYZ+RTMYZ                                               1S0066
      RSUMZZ=RSUMZZ+RTMZZ                                               1S0067
      IF(-ABSF(RSUMXX)*REX+ABSF(RTMXX)-AEX)1,1,6                        1S0068
    1 IF(-ABSF(RSUMXY)*REXY+ABSF(RTMXY)-AEXY)2,2,6                      1S0069
    2 IF(-ABSF(RSUMXZ)*REXZ+ABSF(RTMXZ)-AEXZ)3,3,6                      1S0070
    3 IF(-ABSF(RSUMYY)*REY+ABSF(RTMYY)-AEY)4,4,6                        1S0071
    4 IF(-ABSF(RSUMYZ)*REYZ+ABSF(RTMYZ)-AEYZ)5,5,6                      1S0072
    5 IF(-ABSF(RSUMZZ)*REZ+ABSF(RTMZZ)-AEZ)16,16,6                      1S0073
    6 CONTINUE                                                          1S0074
      BIGO=RTMXX                                                        1S0075
      IF(ABSF(BIGO)-ABSF(RTMXY))7,8,8                                   1S0076
    7 BIGO=RTMXY                                                        1S0077
    8 IF(ABSF(BIGO)-ABSF(RTMXZ))9,10,10                                 1S0078
    9 BIGO=RTMXZ                                                        1S0079
   10 IF(ABSF(BIGO)-ABSF(RTMYY))11,12,12                                1S0080
   11 BIGO=RTMYY                                                        1S0081
   12 IF(ABSF(BIGO)-ABSF(RTMYZ))13,14,14                                1S0082
   13 BIGO=RTMYZ                                                        1S0083
   14 IF(ABSF(BIGO)-ABSF(RTMZZ))15,16,16                                1S0084
   15 BIGO=RTMZZ                                                        1S0085
   16 DO 51 I=1,N                                                       1S0086
      K=1                                                               1S0087
      XMU1=I                                                            1S0088
      HX1=XMU1                                                          1S0089
      HX2=-XMU1                                                         1S0090
      SV1=PV1*XMU1                                                      1S0091
      SV2=CS1*XMU1                                                      1S0092
      SV3=-XMU1*CTGAM                                                   1S0093
      DO 37 J=1,N                                                       1S0094
      XMU2=J                                                            1S0095
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      T22=XMU2*TE                                                       ISO096
      HY1=SV3+T22                                                       ISO097
      HY2=-SV3+T22                                                      ISO098
      H1=SQRTF(HX1*HX1+HY1*HY1)                                         ISO099
      H2=SQRTF(HX2*HX2+HY2*HY2)                                         ISO100
      T31=PV2*XMU2+SV1                                                  ISO101
      T32=PV2*XMU2-SV1                                                  ISO102
      X11=CCSF(T31)                                                     ISO103
      X21=SINF(T31)                                                     ISO104
      X12=CCSF(T32)                                                     ISO105
      X22=SINF(T32)                                                     ISO106
      T41=CS2*XMU2+SV2                                                  ISO107
      T42=CS2*XMU2-SV2                                                  ISO108
      Y11=CCSF(T41)                                                     ISO109
      Y12=CCSF(T42)                                                     ISO110
      Y21=SINF(T41)                                                     ISO111
      Y22=SINF(T42)                                                     ISO112
      W1=EXPF(POW*H1)                                                   ISO113
      W2=EXPF(POW*H2)                                                   ISO114
      Z1=EXPF(POW3*H1)                                                  ISO115
      Z2=EXPF(POW3*H2)                                                  ISO116
      T11=1./Z1                                                         ISO117
      T12=1./Z2                                                         ISO118
      T21=1./W1                                                         ISO119
      T22=1./W2                                                         ISO120
      T31=X11*Y11+X21*Y21                                               ISO121
      T32=X12*Y12+X22*Y22                                               ISO122
      T41=X21*Y11-X11*Y21                                               ISO123
      T42=X22*Y12-X12*Y22                                               ISO124
      T51=-2.*Y11+W1+T21                                                ISO125
      T52=-2.*Y12+W2+T22                                                ISO126
      T61=W1*Z1                                                         ISO127
      T62=W2*Z2                                                         ISO128
      T71=T11*T21                                                       ISO129
      T72=T12*T22                                                       ISO130
      T81=1./T51                                                        ISO131
      T82=1./T52                                                        ISO132
      ROMG31=((Z1-T11)*T31-(T61-T71)*X11)*T81                           ISO133
      ROMG32=((Z2-T12)*T32-(T62-T72)*X12)*T82                           ISO134
      COMG31=((Z1+T11)*T41-(T61+T71)*X21)*T81                           ISO135
      COMG32=((Z2+T12)*T42-(T62+T72)*X22)*T82                           ISO136
      RTMXX=-2.*HX1*HX1*ROMG31/H1-2.*HX2*HX2*ROMG32/H2                  ISO137
      RTMXY=-2.*HX1*HY1*ROMG31/H1-2.*HX2*HY2*ROMG32/H2                  ISO138
      RTMXZ=-2.*HX1*COMG31-2.*HX2*COMG32                                ISO139
      RTMYY=-2.*HY1*HY1*ROMG31/H1-2.*HY2*HY2*ROMG32/H2                  ISO140
      RTMYZ=-2.*HY1*COMG31-2.*HY2*COMG32                                ISO141
      RTMZZ=2.*H1*ROMG31+2.*H2*ROMG32                                   ISO142
      RSUMXX=RSUMXX+RTMXX                                               ISO143
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      RSUMXY=RSUMXY+RTMXY                                                    1S0144
      RSUMXZ=RSUMXZ+RTMXZ                                                    1S0145
      RSUMYY=RSUMYY+RTMYY                                                    1S0146
      RSUMYZ=RSUMYZ+RTMYZ                                                    1S0147
      RSUMZZ=RSUMZZ+RTMZZ                                                    1S0148
      IF(-ABSF(RSUMXX)*REX+ABSF(RTMXX)-AEX)26,26,37                          1S0149
   26 IF(-ABSF(RSUMXY)*REXY+ABSF(RTMXY)-AEXY)27,27,37                        1S0150
   27 IF(-ABSF(RSUMXZ)*REXZ+ABSF(RTMXZ)-AEXZ)28,28,37                        1S0151
   28 IF(-ABSF(RSUMYY)*REY+ABSF(RTMYY)-AEY)29,29,37                          1S0152
   29 IF(-ABSF(RSUMYZ)*REYZ+ABSF(RTMYZ)-AEYZ)30,30,37                        1S0153
   30 IF(-ABSF(RSUMZZ)*REZ+ABSF(RTMZZ)-AEZ)31,31,37                          1S0154
   31 IF(J-I)36,32,32                                                        1S0155
   32 IF(J-JIG)37,33,33                                                      1S0156
   33 IF(J-I)36,35,51                                                        1S0157
   35 IF(K-I)51,52,52                                                        1S0158
   36 K=K+1                                                                  1S0159
   37 CONTINUE                                                               1S0160
      LINE2=I                                                                1S0161
      IF(LINE1)38,38,39                                                      1S0162
   38 LINE1=I                                                                1S0163
   39 L=L+1                                                                  1S0164
      IF(ABSF(BIG)-ABSF(RTMXX))40,41,41                                      1S0165
   40 BIG=RTMXX                                                              1S0166
   41 IF(ABSF(BIG)-ABSF(RTMXY))42,43,43                                      1S0167
   42 BIG=RTMXY                                                              1S0168
   43 IF(ABSF(BIG)-ABSF(RTMXZ))44,45,45                                      1S0169
   44 BIG=RTMXZ                                                              1S0170
   45 IF(ABSF(BIG)-ABSF(RTMYY))46,47,47                                      1S0171
   46 BIG=RTMYY                                                              1S0172
   47 IF(ABSF(BIG)-ABSF(RTMYZ))48,49,49                                      1S0173
   48 BIG=RTMYZ                                                              1S0174
   49 IF(ABSF(BIG)-ABSF(RTMZZ))50,51,51                                      1S0175
   50 BIG=RTMZZ                                                              1S0176
   51 CONTINUE                                                               1S0177
      M=1                                                                    1S0178
   52 SUMXX=AMP*RSUMXX                                                       1S0179
      SUMXY=AMP*RSUMXY                                                       1S0180
      SUMXZ=AMP*RSUMXZ                                                       1S0181
      SUMYY=AMP*RSUMYY                                                       1S0182
      SUMYZ=AMP*RSUMYZ                                                       1S0183
      SUMZZ=AMP*RSUMZZ                                                       1S0184
      BIGO=BIGO*AMP                                                          1S0185
      BIG=BIG*AMP                                                            1S0186
      RETURN                                                                 1S0187
      END                                                                    1S0188
```

```
 SUBROUTINE SUM2                                                                2S0000
0COMMON A1,A2,A3,XJ1,XJ2,XJ3,XALPH,XBET,XGAM,XDEL,AEX,REX,AEY,REY,A             2S0001
1EZ,REZ,AEXY,REXY,AEXZ,REXZ,AEYZ,REYZ,L,M,N,LL,MM,LINE1,LINE2,NILE1            2S0002
2,NILE2,MIRE,BIGO,BIG,CIGO,CIG,RTMXX,RTMXY,RTMXZ,RTMYY,RTMYZ,RTMZZ,            2S0003
3RSUMXX,RSUMXY,RSUMXZ,RSUMYY,RSUMYZ,RSUMZZ,SUMXX,SUMXY,SUMXZ,SUMYY,            2S0004
4SUMYZ,SUMZZ,PI,SPI,SIGAM,CTGAM,COGAM,COALPH,COBET,COCEL,SICEL,OA,V             2S0005
5OL,POW,POW3,PV1,PV2,TE,CS1,CS2,AMP,JIG,XSI1,XSI2,ADD,RATIO,XMU1,XM            2S0006
6U2,S1,S2,SV1,SV2,SV3,H1,H2,HX1,HX2,HY1,HY2,W1,W2,Z1,Z2,X11,X12,X21            2S0007
7,X22,Y11,Y12,Y21,Y22,ROMG31,ROMG32,COMG31,COMG32,GP11,GP12,GM11,GM            2S0008
812,GP31,GP32,GP51,GP52,T11,T12,T21,T22,T31,T32,T41,T42,T51,T52,T61            2S0009
9,T62,T71,T72,T81,T82                                                          2S0010
 MIRE=2                                                                        2S0011
 DO 6 I=1,N                                                                    2S0012
 XMU1=I                                                                        2S0013
 H1=XMU1/SIGAM                                                                 2S0014
 T11=PV1*XMU1                                                                  2S0015
 X11=CCSF(T11)                                                                 2S0016
 X21=SINF(T11)                                                                 2S0017
 W1=EXPF(POW*H1)                                                               2S0018
 Z1=EXPF(-POW3*H1)                                                             2S0019
 T11=W1/Z1                                                                     2S0020
 T21=1./(1.-W1)                                                                2S0021
 ROMG31=X11*T21*(T11+Z1)                                                       2S0022
 COMG31=X21*T21*(T11-Z1)                                                       2S0023
 RTMXX=-2.*XMU1*SIGAM*ROMG31                                                   2S0024
 RTMXY=-RTMXX*CTGAM                                                            2S0025
 RTMXZ=-2.*XMU1*COMG31                                                         2S0026
 RTMYY=CTGAM*CTGAM*RTMXX                                                       2S0027
 RTMYZ=-CTGAM*RTMXZ                                                            2S0028
 RTMZZ=2.*H1*ROMG31                                                            2S0029
 XMU2=XMU1                                                                     2S0030
 H1=XMU2*TE                                                                    2S0031
 T11=PV2*XMU2                                                                  2S0032
 X11=CCSF(T11)                                                                 2S0033
 X21=SINF(T11)                                                                 2S0034
 W1=EXPF(POW*H1)                                                               2S0035
 Z1=EXPF(-POW3*H1)                                                             2S0036
 T11=W1/Z1                                                                     2S0037
 T21=1./(1.-W1)                                                                2S0038
 ROMG31=X11*T21*(T11+Z1)                                                       2S0039
 COMG31=X21*T21*(T11-Z1)                                                       2S0040
 RTMYY=RTMYY-2.*H1*ROMG31                                                      2S0041
 RTMYZ=RTMYZ-2.*H1*COMG31                                                      2S0042
 RTMZZ=RTMZZ+2.*H1*ROMG31                                                      2S0043
 RSUMXX=RSUMXX+RTMXX                                                           2S0044
 RSUMXY=RSUMXY+RTMXY                                                           2S0045
 RSUMXZ=RSUMXZ+RTMXZ                                                           2S0046
 RSUMYY=RSUMYY+RTMYY                                                           2S0047
```

```
      RSUMYZ=RSUMYZ+RTMYZ                                                2S0048
      RSUMZZ=RSUMZZ+RTMZZ                                                2S0049
      IF(-ABSF(RSUMXX)*REX+ABSF(RTMXX)-AEX)1,1,6                         2S0050
    1 IF(-ABSF(RSUMXY)*REXY+ABSF(RTMXY)-AEXY)2,2,6                       2S0051
    2 IF(-ABSF(RSUMXZ)*REXZ+ABSF(RTMXZ)-AEXZ)3,3,6                       2S0052
    3 IF(-ABSF(RSUMYY)*REY+ABSF(RTMYY)-AEY)4,4,6                         2S0053
    4 IF(-ABSF(RSUMYZ)*REYZ+ABSF(RTMYZ)-AEYZ)5,5,6                       2S0054
    5 IF(-ABSF(RSUMZZ)*REZ+ABSF(RTMZZ)-AEZ)16,16,6                       2S0055
    6 CONTINUE                                                           2S0056
      BIGO=RTMXX                                                         2S0057
      IF(ABSF(BIGO)-ABSF(RTMXY))7,8,8                                    2S0058
    7 BIGO=RTMXY                                                         2S0059
    8 IF(ABSF(BIGO)-ABSF(RTMXZ))9,10,10                                  2S0060
    9 BIGO=RTMXZ                                                         2S0061
   10 IF(ABSF(BIGO)-ABSF(RTMYY))11,12,12                                 2S0062
   11 BIGO=RTMYY                                                         2S0063
   12 IF(ABSF(BIGO)-ABSF(RTMYZ))13,14,14                                 2S0064
   13 BIGO=RTMYZ                                                         2S0065
   14 IF(ABSF(BIGO)-ABSF(RTMZZ))15,16,16                                 2S0066
   15 BIGO=RTMZZ                                                         2S0067
   16 DO 51 I=1,N                                                        2S0068
      K=1                                                                2S0069
      XMU1=I                                                             2S0070
      HX1=XMU1                                                           2S0071
      HX2=-XMU1                                                          2S0072
      SV1=PV1*XMU1                                                       2S0073
      SV3=-XMU1*CTGAM                                                    2S0074
      DO 37 J=1,N                                                        2S0075
      XMU2=J                                                             2S0076
      T22=XMU2*TE                                                        2S0077
      HY1=SV3+T22                                                        2S0078
      HY2=-SV3+T22                                                       2S0079
      H1=SQRTF(HX1*HX1+HY1*HY1)                                          2S0080
      H2=SQRTF(HX2*HX2+HY2*HY2)                                          2S0081
      T31=PV2*XMU2+SV1                                                   2S0082
      T32=PV2*XMU2-SV1                                                   2S0083
      X11=CCSF(T31)                                                      2S0084
      X12=CCSF(T32)                                                      2S0085
      X21=SINF(T31)                                                      2S0086
      X22=SINF(T32)                                                      2S0087
      W1=EXPF(POW*H1)                                                    2S0088
      W2=EXPF(POW*H2)                                                    2S0089
      Z1=EXPF(-POW3*H1)                                                  2S0090
      Z2=EXPF(-POW3*H2)                                                  2S0091
      T11=W1/Z1                                                          2S0092
      T12=W2/Z2                                                          2S0093
      T21=1./(1.-W1)                                                     2S0094
      T22=1./(1.-W2)                                                     2S0095
```

```
      ROMG31=X11*T21*(T11+Z1)                                                2S0096
      ROMG32=X12*T22*(T12+Z2)                                                2S0097
      COMG31=X21*T21*(T11-Z1)                                                2S0098
      COMG32=X22*T22*(T12-Z2)                                                2S0099
      RTMXX=-2.*HX1*HX1*ROMG31/H1-2.*HX2*HX2*ROMG32/H2                       2S0100
      RTMXY=-2.*HX1*HY1*ROMG31/H1-2.*HX2*HY2*ROMG32/H2                       2S0101
      RTMXZ=-2.*HX1*COMG31-2.*HX2*COMG32                                     2S0102
      RTMYY=-2.*HY1*HY1*ROMG31/H1-2.*HY2*HY2*ROMG32/H2                       2S0103
      RTMYZ=-2.*HY1*COMG31-2.*HY2*COMG32                                     2S0104
      RTMZZ=2.*H1*ROMG31+2.*H2*ROMG32                                        2S0105
      RSUMXX=RSUMXX+RTMXX                                                    2S0106
      RSUMXY=RSUMXY+RTMXY                                                    2S0107
      RSUMXZ=RSUMXZ+RTMXZ                                                    2S0108
      RSUMYY=RSUMYY+RTMYY                                                    2S0109
      RSUMYZ=RSUMYZ+RTMYZ                                                    2S0110
      RSUMZZ=RSUMZZ+RTMZZ                                                    2S0111
      IF(-ABSF(RSUMXX)*REX+ABSF(RTMXX)-AEX)26,26,37                          2S0112
   26 IF(-ABSF(RSUMXY)*REXY+ABSF(RTMXY)-AEXY)27,27,37                        2S0113
   27 IF(-ABSF(RSUMXZ)*REXZ+ABSF(RTMXZ)-AEXZ)28,28,37                        2S0114
   28 IF(-ABSF(RSUMYY)*REY+ABSF(RTMYY)-AEY)29,29,37                          2S0115
   29 IF(-ABSF(RSUMYZ)*REYZ+ABSF(RTMYZ)-AEYZ)30,30,37                        2S0116
   30 IF(-ABSF(RSUMZZ)*REZ+ABSF(RTMZZ)-AEZ)31,31,37                          2S0117
   31 IF(J-I)36,32,32                                                        2S0118
   32 IF(J-JIG)37,33,33                                                      2S0119
   33 IF(J-I)36,35,51                                                        2S0120
   35 IF(K-I)51,52,52                                                        2S0121
   36 K=K+1                                                                  2S0122
   37 CONTINUE                                                               2S0123
      LINE2=I                                                                2S0124
      IF(LINE1)38,38,39                                                      2S0125
   38 LINE1=I                                                                2S0126
   39 L=L+1                                                                  2S0127
      IF(ABSF(BIG)-ABSF(RTMXX))40,41,41                                      2S0128
   40 BIG=RTMXX                                                              2S0129
   41 IF(ABSF(BIG)-ABSF(RTMXY))42,43,43                                      2S0130
   42 BIG=RTMXY                                                              2S0131
   43 IF(ABSF(BIG)-ABSF(RTMXZ))44,45,45                                      2S0132
   44 BIG=RTMXZ                                                              2S0133
   45 IF(ABSF(BIG)-ABSF(RTMYY))46,47,47                                      2S0134
   46 BIG=RTMYY                                                              2S0135
   47 IF(ABSF(BIG)-ABSF(RTMYZ))48,49,49                                      2S0136
   48 BIG=RTMYZ                                                              2S0137
   49 IF(ABSF(BIG)-ABSF(RTMZZ))50,51,51                                      2S0138
   50 BIG=RTMZZ                                                              2S0139
   51 CONTINUE                                                               2S0140
      M=1                                                                    2S0141
   52 SUMXX=AMP*RSUMXX                                                       2S0142
      SUMXY=AMP*RSUMXY                                                       2S0143
```

```
      SUMXZ=AMP*RSUMXZ                                                  2S0144
      SUMYY=AMP*RSUMYY                                                  2S0145
      SUMYZ=AMP*RSUMYZ                                                  2S0146
      SUMZZ=AMP*RSUMZZ                                                  2S0147
      BIGO=BIGO*AMP                                                     2S0148
      BIG=BIG*AMP                                                       2S0149
      RETURN                                                            2S0150
      END                                                               2S0151
```

```
      SUBROUTINE SUM3                                                   3S0001
     0COMMON A1,A2,A3,XJ1,XJ2,XJ3,XALPH,XBET,XGAM,XDEL,AEX,REX,AEY,REY,A 3S0002
     1EZ,REZ,AEXY,REXY,AEXZ,REXZ,AEYZ,REYZ,L,M,N,LL,MM,LINE1,LINE2,NILE1 3S0003
     2,NILE2,MIRE,BIGO,BIG,CIGO,CIG,RTMXX,RTMXY,RTMXZ,RTMYY,RTMYZ,RTMZZ, 3S0004
     3RSUMXX,RSUMXY,RSUMXZ,RSUMYY,RSUMYZ,RSUMZZ,SUMXX,SUMXY,SUMXZ,SUMYY, 3S0005
     4SUMYZ,SUMZZ,PI,SPI,SIGAM,CTGAM,COGAM,COALPH,COBET,CODEL,SIDEL,OA,V 3S0006
     5OL,POW,POW3,PV1,PV2,TE,CS1,CS2,AMP,JIG,XSI1,XSI2,ADD,RATIO,XMU1,XM 3S0007
     6U2,S1,S2,SV1,SV2,SV3,H1,H2,HX1,HX2,HY1,HY2,W1,W2,Z1,Z2,X11,X12,X21 3S0008
     7,X22,Y11,Y12,Y21,Y22,ROMG31,ROMG32,COMG31,COMG32,GP11,GP12,GM11,GM 3S0009
     812,GP31,GP32,GP51,GP52,T11,T12,T21,T22,T31,T32,T41,T42,T51,T52,T61 3S0010
     9,T62,T71,T72,T81,T82                                              3S0011
      MIRE=3                                                            3S0012
      DO 6 I=1,N                                                        3S0013
      XMU1=I                                                            3S0014
      H1=XMU1/SIGAM                                                     3S0015
      W1=EXPF(POW*H1)                                                   3S0016
      Z1=EXPF(-POW3*H1)                                                 3S0017
      T11=W1/Z1                                                         3S0018
      T21=1./(1.-W1)                                                    3S0019
      ROMG31=T21*(T11+Z1)                                               3S0020
      RTMXX=-2.*XMU1*SIGAM*ROMG31                                       3S0021
      RTMXY=-RTMXX*CTGAM                                                3S0022
      RTMYY=CTGAM*CTGAM*RTMXX                                           3S0023
      RTMZZ=2.*H1*ROMG31                                                3S0024
      XMU2=XMU1                                                         3S0025
      H1=XMU2*TE                                                        3S0026
      W1=EXPF(POW*H1)                                                   3S0027
      Z1=EXPF(-POW3*H1)                                                 3S0028
      T11=W1/Z1                                                         3S0029
      T21=1./(1.-W1)                                                    3S0030
      ROMG31=T21*(T11+Z1)                                               3S0031
      RTMYY=RTMYY-2.*H1*ROMG31                                          3S0032
      RTMZZ=RTMZZ+2.*H1*ROMG31                                          3S0033
      RSUMXX=RSUMXX+RTMXX                                               3S0034
      RSUMXY=RSUMXY+RTMXY                                               3S0035
      RSUMYY=RSUMYY+RTMYY                                               3S0036
      RSUMZZ=RSUMZZ+RTMZZ                                               3S0037
      IF(-ABSF(RSUMXX)*REX+ABSF(RTMXX)-AEX)1,1,6                        3S0038
    1 IF(-ABSF(RSUMXY)*REXY+ABSF(RTMXY)-AEXY)3,3,6                      3S0039
    3 IF(-ABSF(RSUMYY)*REY+ABSF(RTMYY)-AEY)5,5,6                        3S0040
    5 IF(-ABSF(RSUMZZ)*REZ+ABSF(RTMZZ)-AEZ)16,16,6                      3S0041
    6 CONTINUE                                                          3S0042
      BIGO=RTMXX                                                        3S0043
      IF(ABSF(BIGO)-ABSF(RTMXY))7,10,10                                 3S0044
    7 BIGO=RTMXY                                                        3S0045
   10 IF(ABSF(BIGO)-ABSF(RTMYY))11,14,14                                3S0046
   11 BIGO=RTMYY                                                        3S0047
   14 IF(ABSF(BIGO)-ABSF(RTMZZ))15,16,16                                3S0048
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```
15 BIGO=RTMZZ                                                                    3S0049
16 DO 51 I=1,N                                                                   3S0050
   K=1                                                                           3S0051
   XMU1=I                                                                        3S0052
   HX1=XMU1                                                                      3S0053
   HX2=-XMU1                                                                     3S0054
   SV3=-XMU1*CTGAM                                                               3S0055
   DO 37 J=1,N                                                                   3S0056
   XMU2=J                                                                        3S0057
   T22=XMU2*TE                                                                   3S0058
   HY1=SV3+T22                                                                   3S0059
   HY2=-SV3+T22                                                                  3S0060
   H1=SQRTF(HX1*HX1+HY1*HY1)                                                     3S0061
   H2=SQRTF(HX2*HX2+HY2*HY2)                                                     3S0062
   W1=EXPF(POW*H1)                                                               3S0063
   W2=EXPF(POW*H2)                                                               3S0064
   Z1=EXPF(-POW3*H1)                                                             3S0065
   Z2=EXPF(-POW3*H2)                                                             3S0066
   T11=W1/Z1                                                                     3S0067
   T12=W2/Z2                                                                     3S0068
   T21=1./(1.-W1)                                                                3S0069
   T22=1./(1.-W2)                                                                3S0070
   ROMG31=T21*(T11+Z1)                                                           3S0071
   ROMG32=T22*(T12+Z2)                                                           3S0072
   RTMXX=-2.*HX1*HX1*ROMG31/H1-2.*HX2*HX2*ROMG32/H2                              3S0073
   RTMXY=-2.*HX1*HY1*ROMG31/H1-2.*HX2*HY2*ROMG32/H2                              3S0074
   RTMYY=-2.*HY1*HY1*ROMG31/H1-2.*HY2*HY2*ROMG32/H2                              3S0075
   RTMZZ=2.*H1*ROMG31+2.*H2*ROMG32                                               3S0076
   RSUMXX=RSUMXX+RTMXX                                                           3S0077
   RSUMXY=RSUMXY+RTMXY                                                           3S0078
   RSUMYY=RSUMYY+RTMYY                                                           3S0079
   RSUMZZ=RSUMZZ+RTMZZ                                                           3S0080
   IF(-ABSF(RSUMXX)*REX+ABSF(RTMXX)-AEX)26,26,37                                 3S0081
26 IF(-ABSF(RSUMXY)*REXY+ABSF(RTMXY)-AEXY)28,28,37                               3S0082
28 IF(-ABSF(RSUMYY)*REY+ABSF(RTMYY)-AEY)30,30,37                                 3S0083
30 IF(-ABSF(RSUMZZ)*REZ+ABSF(RTMZZ)-AEZ)31,31,37                                 3S0084
31 IF(J-I)36,32,32                                                               3S0085
32 IF(J-JIG)37,33,33                                                             3S0086
33 IF(J-I)36,35,51                                                               3S0087
35 IF(K-I)51,52,52                                                               3S0088
36 K=K+1                                                                         3S0089
37 CONTINUE                                                                      3S0090
   LINE2=I                                                                       3S0091
   IF(LINE1)38,38,39                                                             3S0092
38 LINE1=I                                                                       3S0093
39 L=L+1                                                                         3S0094
   IF(ABSF(BIG)-ABSF(RTMXX))40,41,41                                             3S0095
40 BIG=RTMXX                                                                     3S0096
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```
41  IF(ABSF(BIG)-ABSF(RTMXY))42,45,45                                3S0097
42  BIG=RTMXY                                                        3S0098
45  IF(ABSF(BIG)-ABSF(RTMYY))46,49,49                                3S0099
46  BIG=RTMYY                                                        3S0100
49  IF(ABSF(BIG)-ABSF(RTMZZ))50,51,51                                3S0101
50  BIG=RTMZZ                                                        3S0102
51  CONTINUE                                                         3S0103
    M=1                                                              3S0104
52  SUMXX=AMP*RSUMXX                                                 3S0105
    SUMXY=AMP*RSUMXY                                                 3S0106
    SUMYY=AMP*RSUMYY                                                 3S0107
    SUMZZ=AMP*RSUMZZ                                                 3S0108
    BIGO=BIGO*AMP                                                    3S0109
    BIG=BIG*AMP                                                      3S0110
    RETURN                                                           3S0111
    END                                                              3S0112
```

```
 SUBROUTINE SUM4                                                                4S0001
0COMMON A1,A2,A3,XJ1,XJ2,XJ3,XALPH,XBET,XGAM,XDEL,AEX,REX,AEY,REY,A             4S0002
1EZ,REZ,AEXY,REXY,AEXZ,REXZ,AEYZ,REYZ,L,M,N,LL,MM,LINE1,LINE2,NILE1            4S0003
2,NILE2,MIRE,BIGO,BIG,CIGO,CIG,RTMXX,RTMXY,RTMXZ,RTMYY,RTMYZ,RTMZZ,            4S0004
3RSUMXX,RSUMXY,RSUMXZ,RSUMYY,RSUMYZ,RSUMZZ,SUMXX,SUMXY,SUMXZ,SUMYY,            4S0005
4SUMYZ,SUMZZ,PI,SPI,SIGAM,CTGAM,COGAM,CCALPH,CCBET,CODEL,SIDEL,CA,V             4S0006
5OL,POW,POW3,PV1,PV2,TE,CS1,CS2,AMP,JIG,XSI1,XSI2,ADD,RATIO,XMU1,XM             4S0007
6U2,S1,S2,SV1,SV2,SV3,H1,H2,HX1,HX2,HY1,HY2,W1,W2,Z1,Z2,X11,X12,X21             4S0008
7,X22,Y11,Y12,Y21,Y22,ROMG31,ROMG32,COMG31,COMG32,GP11,GP12,GM11,GM             4S0009
812,GP31,GP32,GP51,GP52,T11,T12,T21,T22,T31,T32,T41,T42,T51,T52,T61            4S0010
9,T62,T71,T72,T81,T82                                                          4S0011
 MIRE=4                                                                        4S0012
 H2=0.                                                                         4S0013
 TANG=-1./SPI                                                                  4S0014
 DO 6 I=1,N                                                                    4S0015
 XMU1=I                                                                        4S0016
 H1=XMU1/SIGAM                                                                 4S0017
 T11=PV1*XMU1                                                                  4S0018
 X11=CCSF(T11)                                                                 4S0019
 T11=CS1*XMU1                                                                  4S0020
 Y11=CCSF(T11)                                                                 4S0021
 Y21=SINF(T11)                                                                 4S0022
 W1=EXPF(-POW*H1)                                                              4S0023
 T11=1./W1                                                                     4S0024
 T21=1./(W1-2.*Y11+T11)                                                        4S0025
 ROMG31=(Y11-T11)*2.*X11*T21                                                   4S0026
 COMG31=-2.*X11*Y21*T21                                                        4S0027
 CALL GAM1                                                                     4S0028
 RTMXX=-2.*XMU1*SIGAM*ROMG31+TANG*X11*((2.*XMU1*SIGAM-H1)*GP11-0.5*            4S0029
1H1*GM11)                                                                      4S0030
 RTMXY=2.*XMU1*COGAM*ROMG31-2.*TANG*XMU1*CCGAM*X11*GP11                        4S0031
 RTMXZ=-2.*XMU1*COMG31                                                         4S0032
 RTMYY=-2.*XMU1*COGAM*CTGAM*ROMG31+TANG*X11*((2.*XMU1*CCGAM*CTGAM-H            4S0033
11)*GP11-0.5*H1*GM11)                                                          4S0034
 RTMYZ=-CTGAM*RTMXZ                                                            4S0035
 RTMZZ=2.*H1*ROMG31+TANG*H1*X11*GM11                                           4S0036
 XMU2=XMU1                                                                     4S0037
 H1=XMU2*TE                                                                    4S0038
 T11=PV2*XMU2                                                                  4S0039
 X11=CCSF(T11)                                                                 4S0040
 T11=CS2*XMU2                                                                  4S0041
 Y11=CCSF(T11)                                                                 4S0042
 Y21=SINF(T11)                                                                 4S0043
 W1=EXPF(-POW*H1)                                                              4S0044
 T11=1./W1                                                                     4S0045
 T21=1./(W1-2.*Y11+T11)                                                        4S0046
 ROMG31=(Y11-T11)*2.*X11*T21                                                   4S0047
 COMG31=-2.*X11*Y21*T21                                                        4S0048
```

```
      CALL GAM1                                                          4S0049
      RTMXX=RTMXX-TANG*H1*X11*(GP11+0.5*GM11)                            4S0050
      RTMYY=RTMYY-2.*H1*ROMG31+TANG*H1*X11*(GP11-0.5*GM11)               4S0051
      RTMYZ=RTMYZ-2.*H1*COMG31                                           4S0052
      RTMZZ=RTMZZ+2.*H1*ROMG31+TANG*H1*X11*GM11                          4S0053
      RSUMXX=RSUMXX+RTMXX                                                4S0054
      RSUMXY=RSUMXY+RTMXY                                                4S0055
      RSUMXZ=RSUMXZ+RTMXZ                                                4S0056
      RSUMYY=RSUMYY+RTMYY                                                4S0057
      RSUMYZ=RSUMYZ+RTMYZ                                                4S0058
      RSUMZZ=RSUMZZ+RTMZZ                                                4S0059
      IF(-ABSF(RSUMXX)*REX+ABSF(RTMXX)-AEX)1,1,6                         4S0060
    1 IF(-ABSF(RSUMXY)*REXY+ABSF(RTMXY)-AEXY)2,2,6                       4S0061
    2 IF(-ABSF(RSUMXZ)*REXZ+ABSF(RTMXZ)-AEXZ)3,3,6                       4S0062
    3 IF(-ABSF(RSUMYY)*REY+ABSF(RTMYY)-AEY)4,4,6                         4S0063
    4 IF(-ABSF(RSUMYZ)*REYZ+ABSF(RTMYZ)-AEYZ)5,5,6                       4S0064
    5 IF(-ABSF(RSUMZZ)*REZ+ABSF(RTMZZ)-AEZ)16,16,6                       4S0065
    6 CONTINUE                                                           4S0066
      BIGO=RTMXX                                                         4S0067
      IF(ABSF(BIGO)-ABSF(RTMXY))7,8,8                                    4S0068
    7 BIGO=RTMXY                                                         4S0069
    8 IF(ABSF(BIGO)-ABSF(RTMXZ))9,10,10                                  4S0070
    9 BIGO=RTMXZ                                                         4S0071
   10 IF(ABSF(BIGO)-ABSF(RTMYY))11,12,12                                 4S0072
   11 BIGO=RTMYY                                                         4S0073
   12 IF(ABSF(BIGO)-ABSF(RTMYZ))13,14,14                                 4S0074
   13 BIGO=RTMYZ                                                         4S0075
   14 IF(ABSF(BIGO)-ABSF(RTMZZ))15,16,16                                 4S0076
   15 BIGO=RTMZZ                                                         4S0077
   16 DO 51 I=1,N                                                        4S0078
      K=1                                                                4S0079
      XMU1=I                                                             4S0080
      HX1=XMU1                                                           4S0081
      HX2=-XMU1                                                          4S0082
      SV1=PV1*XMU1                                                       4S0083
      SV2=CS1*XMU1                                                       4S0084
      SV3=-XMU1*CTGAM                                                    4S0085
      DO 37 J=1,N                                                        4S0086
      XMU2=J                                                             4S0087
      T22=XMU2*TE                                                        4S0088
      HY1=SV3+T22                                                        4S0089
      HY2=-SV3+T22                                                       4S0090
      H1=SQRTF(HX1*HX1+HY1*HY1)                                          4S0091
      H2=SQRTF(HX2*HX2+HY2*HY2)                                          4S0092
      T31=PV2*XMU2+SV1                                                   4S0093
      T32=PV2*XMU2-SV1                                                   4S0094
      X11=CCSF(T31)                                                      4S0095
      X12=CCSF(T32)                                                      4S0096
```

```
      T41=CS2*XMU2+SV2                                                          4S0097
      T42=CS2*XMU2-SV2                                                          4S0098
      Y11=CCSF(T41)                                                             4S0099
      Y12=CCSF(T42)                                                             4S0100
      Y21=SINF(T41)                                                             4S0101
      Y22=SINF(T42)                                                             4S0102
      W1=EXPF(-POW*H1)                                                          4S0103
      W2=EXPF(-POW*H2)                                                          4S0104
      T11=1./W1                                                                 4S0105
      T12=1./W2                                                                 4S0106
      T21=1./(W1-2.*Y11+T11)                                                    4S0107
      T22=1./(W2-2.*Y12+T12)                                                    4S0108
      ROMG31=(Y11-T11)*2.*X11*T21                                               4S0109
      ROMG32=(Y12-T12)*2.*X12*T22                                               4S0110
      COMG31=-2.*X11*Y21*T21                                                    4S0111
      COMG32=-2.*X12*Y22*T22                                                    4S0112
      CALL CAM1                                                                 4S0113
      RTMXX=-2.*HX1*HX1*ROMG31/H1-2.*HX2*HX2*ROMG32/H2+TANG*(X11*((2.*HX        4S0114
     11*HX1/H1-H1)*GP11-0.5*H1*GM11)+X12*((2.*HX2*HX2/H2-H2)*GP12-0.5*H2        4S0115
     2*GM12))                                                                   4S0116
      RTMXY=-2.*HX1*HY1*ROMG31/H1-2.*HX2*HY2*ROMG32/H2+2.*TANG*(HX1*HY1*        4S0117
     1X11*GP11/H1+HX2*HY2*X12*GP12/H2)                                          4S0118
      RTMXZ=-2.*HX1*COMG31-2.*HX2*COMG32                                        4S0119
      RTMYY=-2.*HY1*HY1*ROMG31/H1-2.*HY2*HY2*ROMG32/H2+TANG*(X11*((2.*HY        4S0120
     11*HY1/H1-H1)*GP11-0.5*H1*GM11)+X12*((2.*HY2*HY2/H2-H2)*GP12-0.5*H2        4S0121
     2*GM12))                                                                   4S0122
      RTMYZ=-2.*HY1*COMG31-2.*HY2*COMG32                                        4S0123
      RTMZZ=2.*H1*ROMG31+2.*H2*ROMG32+TANG*(H1*GM11*X11+H2*GM12*X12)            4S0124
      RSUMXX=RSUMXX+RTMXX                                                       4S0125
      RSUMXY=RSUMXY+RTMXY                                                       4S0126
      RSUMXZ=RSUMXZ+RTMXZ                                                       4S0127
      RSUMYY=RSUMYY+RTMYY                                                       4S0128
      RSUMYZ=RSUMYZ+RTMYZ                                                       4S0129
      RSUMZZ=RSUMZZ+RTMZZ                                                       4S0130
      IF(-ABSF(RSUMXX)*REX+ABSF(RTMXX)-AEX)26,26,37                             4S0131
   26 IF(-ABSF(RSUMXY)*REXY+ABSF(RTMXY)-AEXY)27,27,37                           4S0132
   27 IF(-ABSF(RSUMXZ)*REXZ+ABSF(RTMXZ)-AEXZ)28,28,37                           4S0133
   28 IF(-ABSF(RSUMYY)*REY+ABSF(RTMYY)-AEY)29,29,37                             4S0134
   29 IF(-ABSF(RSUMYZ)*REYZ+ABSF(RTMYZ)-AEYZ)30,30,37                           4S0135
   30 IF(-ABSF(RSUMZZ)*REZ+ABSF(RTMZZ)-AEZ)31,31,37                             4S0136
   31 IF(J-I)36,32,32                                                           4S0137
   32 IF(J-JIG)37,33,33                                                         4S0138
   33 IF(J-I)36,35,51                                                           4S0139
   35 IF(K-I)51,52,52                                                           4S0140
   36 K=K+1                                                                     4S0141
   37 CONTINUE                                                                  4S0142
      LINE2=I                                                                   4S0143
      IF(LINE1)38,38,39                                                         4S0144
```

```
38 LINE1=I                                                              4S0145
39 L=L+1                                                                4S0146
   IF(ABSF(BIG)-ABSF(RTMXX))40,41,41                                    4S0147
40 BIG=RTMXX                                                            4S0148
41 IF(ABSF(BIG)-ABSF(RTMXY))42,43,43                                    4S0149
42 BIG=RTMXY                                                            4S0150
43 IF(ABSF(BIG)-ABSF(RTMXZ))44,45,45                                    4S0151
44 BIG=RTMXZ                                                            4S0152
45 IF(ABSF(BIG)-ABSF(RTMYY))46,47,47                                    4S0153
46 BIG=RTMYY                                                            4S0154
47 IF(ABSF(BIG)-ABSF(RTMYZ))48,49,49                                    4S0155
48 BIG=RTMYZ                                                            4S0156
49 IF(ABSF(BIG)-ABSF(RTMZZ))50,51,51                                    4S0157
50 BIG=RTMZZ                                                            4S0158
51 CONTINUE                                                             4S0159
   M=1                                                                  4S0160
52 SUMXX=AMP*(RSUMXX+0.5/PI)                                            4S0161
   SUMXY=AMP*RSUMXY                                                     4S0162
   SUMXZ=AMP*RSUMXZ                                                     4S0163
   SUMYY=AMP*(RSUMYY+0.5/PI)                                            4S0164
   SUMYZ=AMP*RSUMYZ                                                     4S0165
   SUMZZ=AMP*(RSUMZZ-1./PI)                                             4S0166
   BIGO=BIGO*AMP                                                        4S0167
   BIG=BIG*AMP                                                          4S0168
   RETURN                                                               4S0169
   END                                                                  4S0170
```

```
      SUBROUTINE SUM5                                                   5S0001
     0COMMON A1,A2,A3,XJ1,XJ2,XJ3,XALPH,XBET,XGAM,XDEL,AEX,REX,AEY,REY,A 5S0002
     1EZ,REZ,AEXY,REXY,AEXZ,REXZ,AEYZ,REYZ,L,M,N,LL,MM,LINE1,LINE2,NILE1 5S0003
     2,NILE2,MIRE,BIGO,BIG,CIGO,CIG,RTMXX,RTMXY,RTMXZ,RTMYY,RTMYZ,RTMZZ, 5S0004
     3RSUMXX,RSUMXY,RSUMXZ,RSUMYY,RSUMYZ,RSUMZZ,SUMXX,SUMXY,SUMXZ,SUMYY, 5S0005
     4SUMYZ,SUMZZ,PI,SPI,SIGAM,CTGAM,COGAM,COALPH,COBET,CODEL,SIDEL,OA,V 5S0006
     5OL,POW,POW3,PV1,PV2,TE,CS1,CS2,AMP,JIG,XSI1,XSI2,ADD,RATIO,XMU1,XM 5S0007
     6U2,S1,S2,SV1,SV2,SV3,H1,H2,HX1,HX2,HY1,HY2,W1,W2,Z1,Z2,X11,X12,X21 5S0008
     7,X22,Y11,Y12,Y21,Y22,ROMG31,ROMG32,COMG31,COMG32,GP11,GP12,GM11,GM 5S0009
     812,GP31,GP32,GP51,GP52,T11,T12,T21,T22,T31,T32,T41,T42,T51,T52,T61 5S0010
     9,T62,T71,T72,T81,T82                                              5S0011
      MIRE=6                                                            5S0012
      H2=0.                                                             5S0013
      TANG=-1./SPI                                                      5S0014
      DO 6 I=1,N                                                        5S0015
      XMU1=I                                                            5S0016
      H1=XMU1/SIGAM                                                     5S0017
      T11=PV1*XMU1                                                      5S0018
      X11=CCSF(T11)                                                     5S0019
      W1=EXPF(-POW*H1)                                                  5S0020
      ROMG31=2.*X11/(W1-1.)                                             5S0021
      CALL GAM1                                                         5S0022
      RTMXX=-2.*XMU1*SIGAM*ROMG31+TANG*X11*((2.*XMU1*SIGAM-H1)*GP11-0.5* 5S0023
     1H1*GM11)                                                          5S0024
      RTMXY=2.*XMU1*COGAM*ROMG31-2.*TANG*XMU1*COGAM*X11*GP11            5S0025
      RTMYY=-2.*XMU1*COGAM*CTGAM*ROMG31+TANG*X11*((2.*XMU1*COGAM*CTGAM-H 5S0026
     11)*GP11-0.5*H1*GM11)                                              5S0027
      RTMZZ=2.*H1*ROMG31+TANG*H1*X11*GM11                               5S0028
      XMU2=XMU1                                                         5S0029
      H1=XMU2*TE                                                        5S0030
      T11=PV2*XMU2                                                      5S0031
      X11=CCSF(T11)                                                     5S0032
      W1=EXPF(-POW*H1)                                                  5S0033
      ROMG31=2.*X11/(W1-1.)                                             5S0034
      CALL GAM1                                                         5S0035
      RTMXX=RTMXX-TANG*H1*X11*(GP11+0.5*GM11)                           5S0036
      RTMYY=RTMYY-2.*H1*ROMG31+TANG*H1*X11*(GP11-0.5*GM11)              5S0037
      RTMZZ=RTMZZ+2.*H1*ROMG31+TANG*H1*X11*GM11                         5S0038
      RSUMXX=RSUMXX+RTMXX                                               5S0039
      RSUMXY=RSUMXY+RTMXY                                               5S0040
      RSUMYY=RSUMYY+RTMYY                                               5S0041
      RSUMZZ=RSUMZZ+RTMZZ                                               5S0042
      IF(-ABSF(RSUMXX)*REX+ABSF(RTMXX)-AEX)1,1,6                        5S0043
    1 IF(-ABSF(RSUMXY)*REXY+ABSF(RTMXY)-AEXY)3,3,6                      5S0044
    3 IF(-ABSF(RSUMYY)*REY+ABSF(RTMYY)-AEY)5,5,6                        5S0045
    5 IF(-ABSF(RSUMZZ)*REZ+ABSF(RTMZZ)-AEZ)16,16,6                      5S0046
    6 CONTINUE                                                          5S0047
      BIGO=RTMXX                                                        5S0048
```

```
      IF(ABSF(BIGO)-ABSF(RTMXY))7,10,10                                 5S0049
    7 BIGO=RTMXY                                                        5S0050
   10 IF(ABSF(BIGO)-ABSF(RTMYY))11,14,14                                5S0051
   11 BIGO=RTMYY                                                        5S0052
   14 IF(ABSF(BIGO)-ABSF(RTMZZ))15,16,16                                5S0053
   15 BIGO=RTMZZ                                                        5S0054
   16 DO 51 I=1,N                                                       5S0055
      K=1                                                               5S0056
      XMU1=I                                                            5S0057
      HX1=XMU1                                                          5S0058
      HX2=-XMU1                                                         5S0059
      SV1=PV1*XMU1                                                      5S0060
      SV2=CS1*XMU1                                                      5S0061
      SV3=-XMU1*CTGAM                                                   5S0062
      DO 37 J=1,N                                                       5S0063
      XMU2=J                                                            5S0064
      T22=XMU2*TE                                                       5S0065
      HY1=SV3+T22                                                       5S0066
      HY2=-SV3+T22                                                      5S0067
      H1=SQRTF(HX1*HX1+HY1*HY1)                                         5S0068
      H2=SQRTF(HX2*HX2+HY2*HY2)                                         5S0069
      T31=PV2*XMU2+SV1                                                  5S0070
      T32=PV2*XMU2-SV1                                                  5S0071
      X11=COSF(T31)                                                     5S0072
      X12=COSF(T32)                                                     5S0073
      W1=EXPF(-POW*H1)                                                  5S0074
      W2=EXPF(-POW*H2)                                                  5S0075
      ROMG31=2.*X11/(W1-1.)                                             5S0076
      ROMG32=2.*X12/(W2-1.)                                             5S0077
      CALL GAM1                                                         5S0078
      RTMXX=-2.*HX1*HX1*ROMG31/H1-2.*HX2*HX2*ROMG32/H2+TANG*(X11*((2.*HX 5S0079
     11*HX1/H1-H1)*GP11-0.5*H1*GM11)+X12*((2.*HX2*HX2/H2-H2)*GP12-0.5*H2 5S0080
     22*GM12))                                                          5S0081
      RTMXY=-2.*HX1*HY1*ROMG31/H1-2.*HX2*HY2*ROMG32/H2+2.*TANG*(HX1*HY1* 5S0082
     1X11*GP11/H1+HX2*HY2*X12*GP12/H2)                                  5S0083
      RTMYY=-2.*HY1*HY1*ROMG31/H1-2.*HY2*HY2*ROMG32/H2+TANG*(X11*((2.*HY 5S0084
     11*HY1/H1-H1)*GP11-0.5*H1*GM11)+X12*((2.*HY2*HY2/H2-H2)*GP12-0.5*H2 5S0085
     22*GM12))                                                          5S0086
      RTMZZ=2.*H1*ROMG31+2.*H2*ROMG32+TANG*(H1*GM11*X11+H2*GM12*X12)    5S0087
      RSUMXX=RSUMXX+RTMXX                                               5S0088
      RSUMXY=RSUMXY+RTMXY                                               5S0089
      RSUMYY=RSUMYY+RTMYY                                               5S0090
      RSUMZZ=RSUMZZ+RTMZZ                                               5S0091
      IF(-ABSF(RSUMXX)*REX+ABSF(RTMXX)-AEX)26,26,37                     5S0092
   26 IF(-ABSF(RSUMXY)*REXY+ABSF(RTMXY)-AEXY)28,28,37                   5S0093
   28 IF(-ABSF(RSUMYY)*REY+ABSF(RTMYY)-AEY)30,30,37                     5S0094
   30 IF(-ABSF(RSUMZZ)*REZ+ABSF(RTMZZ)-AEZ)31,31,37                     5S0095
   31 IF(J-I)36,32,32                                                   5S0096
```

```
32  IF(J-JIG)37,33,33                                                    5S0097
33  IF(J-I)36,35,51                                                      5S0098
35  IF(K-I)51,52,52                                                      5S0099
36  K=K+1                                                                5S0100
37  CONTINUE                                                             5S0101
    LINE2=I                                                              5S0102
    IF(LINE1)38,38,39                                                    5S0103
38  LINE1=I                                                              5S0104
39  L=L+1                                                                5S0105
    IF(ABSF(BIG)-ABSF(RTMXX))40,41,41                                    5S0106
40  BIG=RTMXX                                                            5S0107
41  IF(ABSF(BIG)-ABSF(RTMXY))42,45,45                                    5S0108
42  BIG=RTMXY                                                            5S0109
45  IF(ABSF(BIG)-ABSF(RTMYY))46,49,49                                    5S0110
46  BIG=RTMYY                                                            5S0111
49  IF(ABSF(BIG)-ABSF(RTMZZ))50,51,51                                    5S0112
50  BIG=RTMZZ                                                            5S0113
51  CONTINUE                                                             5S0114
    M=1                                                                  5S0115
52  SUMXX=AMP*(RSUMXX+0.5/PI)                                            5S0116
    SUMXY=AMP*RSUMXY                                                     5S0117
    SUMYY=AMP*(RSUMYY+0.5/PI)                                            5S0118
    SUMZZ=AMP*(RSUMZZ-1./PI)                                             5S0119
    BIGO=BIGO*AMP                                                        5S0120
    BIG=BIG*AMP                                                          5S0121
    RETURN                                                               5S0122
    END                                                                  5S0123
```

```
      SUBROUTINE SUM6                                                   6S0001
     0COMMON A1,A2,A3,XJ1,XJ2,XJ3,XALPH,XBET,XGAM,XDEL,AEX,REX,AEY,REY,A 6S0002
     1EZ,REZ,AEXY,REXY,AEXZ,REXZ,AEYZ,REYZ,L,M,N,LL,MM,LINE1,LINE2,NILE1 6S0003
     2,NILE2,MIRE,BIGO,BIG,CIGO,CIG,RTMXX,RTMXY,RTMXZ,RTMYY,RTMYZ,RTMZZ, 6S0004
     3RSUMXX,RSUMXY,RSUMXZ,RSUMYY,RSUMYZ,RSUMZZ,SUMXX,SUMXY,SUMXZ,SUMYY, 6S0005
     4SUMYZ,SUMZZ,PI,SPI,SIGAM,CTGAM,COGAM,COALPH,COBET,CODEL,SIDEL,OA,V 6S0006
     5OL,POW,POW3,PV1,PV2,TE,CS1,CS2,AMP,JIG,XSI1,XSI2,ADD,RATIO,XMU1,XM 6S0007
     6U2,S1,S2,SV1,SV2,SV3,H1,H2,HX1,HX2,HY1,HY2,W1,W2,Z1,Z2,X11,X12,X21 6S0008
     7,X22,Y11,Y12,Y21,Y22,ROMG31,ROMG32,COMG31,COMG32,GP11,GP12,GM11,GM 6S0009
     812,GP31,GP32,GP51,GP52,T11,T12,T21,T22,T31,T32,T41,T42,T51,T52,T61 6S0010
     9,T62,T71,T72,T81,T82                                              6S0011
      TIM=2./(VOL*SPI)                                                  6S0012
      T11=AMP/TIM                                                       6S0013
      AEX=AEX*T11                                                       6S0014
      REX=REX*T11                                                       6S0015
      AEY=AEY*T11                                                       6S0016
      REY=REY*T11                                                       6S0017
      AEZ=AEZ*T11                                                       6S0018
      REZ=REZ*T11                                                       6S0019
      AEXY=AEXY*T11                                                     6S0020
      REXY=REXY*T11                                                     6S0021
      AEXZ=AEXZ*T11                                                     6S0022
      REXZ=REXZ*T11                                                     6S0023
      AEYZ=AEYZ*T11                                                     6S0024
      REYZ=REYZ*T11                                                     6S0025
      IF(XJ1+XJ2)1,2,1                                                  6S0026
    1 SX1=XJ1+XJ2*OA*CTGAM                                              6S0027
      SY1=XJ2*OA                                                        6S0028
      S1=SQRTF(SX1*SX1+SY1*SY1)                                         6S0029
      S2=0.                                                             6S0030
      CALL GAM2                                                         6S0031
      T11=1./(S1*S1)                                                    6S0032
      T21=T11/S1                                                        6S0033
      RSUMXX=((2.*SX1*SX1*T11-1.)*GP51+0.5*GP31)*T21                    6S0034
      RSUMXY=2.*SX1*SY1*T11*T21*GP51                                    6S0035
      RSUMYY=((2.*SY1*SY1*T11-1.)*GP51+0.5*GP31)*T21                    6S0036
      RSUMZZ=-GP31*T21                                                  6S0037
      GO TO 3                                                           6S0038
    2 MIRE=MIRE+1                                                       6S0039
      T11=-PI*SPI/3.                                                    6S0040
      RSUMXX=T11                                                        6S0041
      RSUMXY=0.                                                         6S0042
      RSUMYY=T11                                                        6S0043
      RSUMZZ=-2.*T11                                                    6S0044
    3 SV1=XJ2*OA                                                        6S0045
      DO 7 I=1,N                                                        6S0046
      XMU1=I                                                            6S0047
      SX1=SV1*CTGAM+XMU1+XJ1                                            6S0048
```

```
      SX2=-2.*XMU1+SX1                                                  6S0049
      S1=SQRTF(SX1*SX1+SV1*SV1)                                         6S0050
      S2=SQRTF(SX2*SX2+SV1*SV1)                                         6S0051
      CALL GAM2                                                         6S0052
      T11=1./(S1*S1)                                                    6S0053
      T12=1./(S2*S2)                                                    6S0054
      T21=T11/S1                                                        6S0055
      T22=T12/S2                                                        6S0056
      T31=(GP31*T21+GP32*T22)*0.5                                       6S0057
      RTMXX=(2.*SX1*SX1*T11-1.)*GP51*T21+(2.*SX2*SX2*T12-1.)*GP52*T22+T3 6S0058
     11                                                                 6S0059
      RTMXY=(SX1*GP51*T11*T21+SX2*GP52*T12*T22)*2.*SV1                  6S0060
      RTMYY=(2.*SV1*SV1*T11-1.)*GP51*T21+(2.*SV1*SV1*T12-1.)*GP52*T22+T3 6S0061
     11                                                                 6S0062
      RTMZZ=-2.*T31                                                     6S0063
      XMU2=XMU1                                                         6S0064
      SY1=XMU2*OA+SV1                                                   6S0065
      SY2=-XMU2*OA+SV1                                                  6S0066
      SX1=SY1*CTGAM+XJ1                                                 6S0067
      SX2=SY2*CTGAM+XJ1                                                 6S0068
      S1=SQRTF(SX1*SX1+SY1*SY1)                                         6S0069
      S2=SQRTF(SX2*SX2+SY2*SY2)                                         6S0070
      CALL GAM2                                                         6S0071
      T11=1./(S1*S1)                                                    6S0072
      T12=1./(S2*S2)                                                    6S0073
      T21=T11/S1                                                        6S0074
      T22=T12/S2                                                        6S0075
      T31=(GP31*T21+GP32*T22)*0.5                                       6S0076
      RTMXX=RTMXX+(2.*SX1*SX1*T11-1.)*GP51*T21+(2.*SX2*SX2*T12-1.)*GP52* 6S0077
     1T22+T31                                                           6S0078
      RTMXY=RTMXY+2.*(SX1*SY1*GP51*T11*T21+SX2*SY2*GP52*T12*T22)        6S0079
      RTMYY=RTMYY+(2.*SY1*SY1*T11-1.)*GP51*T21+(2.*SY2*SY2*T12-1.)*GP52* 6S0080
     1T22+T31                                                           6S0081
      RTMZZ=RTMZZ-2.*T31                                                6S0082
      RSUMXX=RSUMXX+RTMXX                                               6S0083
      RSUMXY=RSUMXY+RTMXY                                               6S0084
      RSUMYY=RSUMYY+RTMYY                                               6S0085
      RSUMZZ=RSUMZZ+RTMZZ                                               6S0086
      IF(-ABSF(RSUMXX)*REX+ABSF(RTMXX)-AEX)4,4,7                        6S0087
    4 IF(-ABSF(RSUMXY)*REXY+ABSF(RTMXY)-AEXY)5,5,7                      6S0088
    5 IF(-ABSF(RSUMYY)*REY+ABSF(RTMYY)-AEY)6,6,7                        6S0089
    6 IF(-ABSF(RSUMZZ)*REZ+ABSF(RTMZZ)-AEZ)13,13,7                      6S0090
    7 CONTINUE                                                          6S0091
      CIGO=RTMXX                                                        6S0092
      IF(ABSF(CIGO)-ABSF(RTMXY))8,9,9                                   6S0093
    8 CIGO=RTMXY                                                        6S0094
    9 IF(ABSF(CIGO)-ABSF(RTMYY))10,11,11                                6S0095
   10 CIGO=RTMYY                                                        6S0096
```

```
11 IF(ABSF(CIGO)-ABSF(RTMZZ))12,13,13                                    6S0097
12 CIGO=RTMZZ                                                            6S0098
13 DO 41 I=1,N                                                           6S0099
   K=1                                                                   6S0100
   XMU1=I                                                                6S0101
   SV1=XMU1+XJ1                                                          6S0102
   SV2=-XMU1+XJ1                                                         6S0103
   DO 31 J=1,N                                                           6S0104
   XMU2=J                                                                6S0105
   SY1=(XMU2+XJ2)*OA                                                     6S0106
   SY2=(-XMU2+XJ2)*OA                                                    6S0107
   SX1=SY1*CTGAM+SV1                                                     6S0108
   SX2=SY1*CTGAM+SV2                                                     6S0109
   S1=SQRTF(SX1*SX1+SY1*SY1)                                             6S0110
   S2=SQRTF(SX2*SX2+SY1*SY1)                                             6S0111
   CALL GAM2                                                             6S0112
   T11=1./(S1*S1)                                                        6S0113
   T12=1./(S2*S2)                                                        6S0114
   T21=T11/S1                                                            6S0115
   T22=T12/S2                                                            6S0116
   T31=(GP31*T21+GP32*T22)*0.5                                           6S0117
   RTMXX=(2.*SX1*SX1*T11-1.)*GP51*T21+(2.*SX2*SX2*T12-1.)*GP52*T22+T3    6S0118
  11                                                                     6S0119
   RTMXY=(SX1*SY1*GP51*T11*T21+SX2*SY1*GP52*T12*T22)*2.                  6S0120
   RTMYY=(2.*SY1*SY1*T11-1.)*GP51*T21+(2.*SY1*SY1*T12-1.)*GP52*T22+T3    6S0121
  11                                                                     6S0122
   RTMZZ=-2.*T31                                                         6S0123
   SX1=SY2*CTGAM+SV1                                                     6S0124
   SX2=SY2*CTGAM+SV2                                                     6S0125
   S1=SQRTF(SX1*SX1+SY2*SY2)                                             6S0126
   S2=SQRTF(SX2*SX2+SY2*SY2)                                             6S0127
   CALL GAM2                                                             6S0128
   T11=1./(S1*S1)                                                        6S0129
   T12=1./(S2*S2)                                                        6S0130
   T21=T11/S1                                                            6S0131
   T22=T12/S2                                                            6S0132
   T31=(GP31*T21+GP32*T22)*0.5                                           6S0133
   RTMXX=RTMXX+(2.*SX1*SX1*T11-1.)*GP51*T21+(2.*SX2*SX2*T12-1.)*GP52*    6S0134
  1T22+T31                                                               6S0135
   RTMXY=RTMXY+(SX1*SY2*GP51*T11*T21+SX2*SY2*GP52*T12*T22)*2.            6S0136
   RTMYY=RTMYY+(2.*SY2*SY2*T11-1.)*GP51*T21+(2.*SY2*SY2*T12-1.)*GP52*    6S0137
  1T22+T31                                                               6S0138
   RTMZZ=RTMZZ-2.*T31                                                    6S0139
   RSUMXX=RSUMXX+RTMXX                                                   6S0140
   RSUMXY=RSUMXY+RTMXY                                                   6S0141
   RSUMYY=RSUMYY+RTMYY                                                   6S0142
   RSUMZZ=RSUMZZ+RTMZZ                                                   6S0143
   IF(-ABSF(RSUMXX)*REX+ABSF(RTMXX)-AEX)23,23,31                         6S0144
```

```
23  IF(-ABSF(RSUMXY)*REXY+ABSF(RTMXY)-AEXY)24,24,31                    6S0145
24  IF(-ABSF(RSUMYY)*REY+ABSF(RTMYY)-AEY)25,25,31                      6S0146
25  IF(-ABSF(RSUMZZ)*REZ+ABSF(RTMZZ)-AEZ)26,26,31                      6S0147
26  IF(J-I)30,27,27                                                    6S0148
27  IF(J-JIG)31,28,28                                                  6S0149
28  IF(J-I)30,29,41                                                    6S0150
29  IF(K-I)41,42,42                                                    6S0151
30  K=K+1                                                              6S0152
31  CONTINUE                                                           6S0153
    NILE2=I                                                            6S0154
    IF(NILE1)32,32,33                                                  6S0155
32  NILE1=I                                                            6S0156
33  LL=LL+1                                                            6S0157
    IF(ABSF(CIG)-ABSF(RTMXX))34,35,35                                  6S0158
34  CIG=RTMXX                                                          6S0159
35  IF(ABSF(CIG)-ABSF(RTMXY))36,37,37                                  6S0160
36  CIG=RTMXY                                                          6S0161
37  IF(ABSF(CIG)-ABSF(RTMYY))38,39,39                                  6S0162
38  CIG=RTMYY                                                          6S0163
39  IF(ABSF(CIG)-ABSF(RTMZZ))40,41,41                                  6S0164
40  CIG=RTMZZ                                                          6S0165
41  CONTINUE                                                           6S0166
    MM=1                                                               6S0167
42  SUMXX=SUMXX+TIM*RSUMXX                                             6S0168
    SUMXY=SUMXY+TIM*RSUMXY                                             6S0169
    SUMYY=SUMYY+TIM*RSUMYY                                             6S0170
    SUMZZ=SUMZZ+TIM*RSUMZZ                                             6S0171
    CIGO=CIGO*TIM                                                      6S0172
    CIG=CIG*TIM                                                        6S0173
    T11=TIM/AMP                                                        6S0174
    AEX=AEX*T11                                                        6S0175
    REX=REX*T11                                                        6S0176
    AEY=AEY*T11                                                        6S0177
    REY=REY*T11                                                        6S0178
    AEZ=AEZ*T11                                                        6S0179
    REZ=REZ*T11                                                        6S0180
    AEXY=AEXY*T11                                                      6S0181
    REXY=REXY*T11                                                      6S0182
    AEXZ=AEXZ*T11                                                      6S0183
    REXZ=REXZ*T11                                                      6S0184
    AEYZ=AEYZ*T11                                                      6S0185
    REYZ=REYZ*T11                                                      6S0186
    RETURN                                                             6S0187
    END                                                                6S0188
```

```
      SUBROUTINE GAM1                                                   1GO0001
     0COMMON A1,A2,A3,XJ1,XJ2,XJ3,XALPH,XBET,XGAM,XDEL,AEX,REX,AEY,REY,A 1GO0002
     1EZ,REZ,AEXY,REXY,AEXZ,REXZ,AEYZ,REYZ,L,M,N,LL,MM,LINE1,LINE2,NILE1 1GO0003
     2,NILE2,MIRE,BIGO,BIG,CIGO,CIG,RTMXX,RTMXY,RTMXZ,RTMYY,RTMYZ,RTMZZ, 1GO0004
     3RSUMXX,RSUMXY,RSUMXZ,RSUMYY,RSUMYZ,RSUMZZ,SUMXX,SUMXY,SUMXZ,SUMYY, 1GO0005
     4SUMYZ,SUMZZ,PI,SPI,SIGAM,CTGAM,COGAM,COALPH,COBET,CODEL,SIDEL,CA,V 1GO0006
     5OL,POW,POW3,PV1,PV2,TE,CS1,CS2,AMP,JIG,XSI1,XSI2,ADD,RATIO,XMU1,XM 1GO0007
     6U2,S1,S2,SV1,SV2,SV3,H1,H2,HX1,HX2,HY1,HY2,W1,W2,Z1,Z2,X11,X12,X21 1GO0008
     7,X22,Y11,Y12,Y21,Y22,ROMG31,ROMG32,COMG31,COMG32,GP11,GP12,GM11,GM 1GO0009
     812,GP31,GP32,GP51,GP52,T11,T12,T21,T22,T31,T32,T41,T42,T51,T52,T61 1GO0010
     9,T62,T71,T72,T81,T82                                              1GO0011
      DIMENSION C(17)                                                   1GO0012
      COMMON C                                                          1GO0013
      IF(H1)1,1,2                                                       1GO0014
    1 GP11=SPI                                                          1GO0015
      GM11=-2.*SPI                                                      1GO0016
      GO TO 9                                                           1GO0017
    2 TRY=-PI*H1*H1                                                     1GO0018
      T71=SPI*H1                                                        1GO0019
      T81=EXPF(TRY)                                                     1GO0020
      IF(TRY+3.)5,3,3                                                   1GO0021
    3 TERM=-2.*T71                                                      1GO0022
      GP11=SPI+TERM                                                     1GO0023
      DO 4 II=1,40                                                      1GO0024
      A=II                                                              1GO0025
      TERM=TERM*TRY*(A-0.5)/(A*(A+0.5))                                 1GO0026
    4 GP11=GP11+TERM                                                    1GO0027
      GO TO 8                                                           1GO0028
    5 X=-3./TRY                                                         1GO0029
      SUM=C(1)                                                          1GO0030
      DO 7 II=2,17                                                      1GO0031
    7 SUM=SUM*X+C(II)                                                   1GO0032
      GP11=SUM*T81/T71                                                  1GO0033
    8 GM11=(T81/T71-GP11)*2.                                            1GO0034
    9 IF(H2)11,11,12                                                    1GO0035
   11 GP12=SPI                                                          1GO0036
      GM12=-2.*SPI                                                      1GO0037
      GO TO 19                                                          1GO0038
   12 TRY=-PI*H2*H2                                                     1GO0039
      T72=SPI*H2                                                        1GO0040
      T82=EXPF(TRY)                                                     1GO0041
      IF(TRY+3.)15,13,13                                                1GO0042
   13 TERM=-2.*T72                                                      1GO0043
      GP12=SPI+TERM                                                     1GO0044
```

```
      DO 14 II=1,40                                                    1G0045
      A=II                                                             1G0046
      TERM=TERM*TRY*(A-0.5)/(A*(A+0.5))                                1G0047
   14 GP12=GP12+TERM                                                   1G0048
      GO TO 18                                                         1G0049
   15 X=-3./TRY                                                        1G0050
      SUM=C(1)                                                         1G0051
      DO 17 II=2,17                                                    1G0052
   17 SUM=SUM*X+C(II)                                                  1G0053
      GP12=SUM*T82/T72                                                 1G0054
   18 GM12=(T82/T72-GP12)*2.                                           1G0055
   19 RETURN                                                           1G0056
      END                                                              1G0057
```

```
      SUBROUTINE GAM2                                                   2G0001
     0COMMON A1,A2,A3,XJ1,XJ2,XJ3,XALPH,XBET,XGAM,XDEL,AEX,REX,AEY,REY,A 2G0002
     1EZ,REZ,AEXY,REXY,AEXZ,REXZ,AEYZ,REYZ,L,M,N,LL,MM,LINE1,LINE2,NILE1 2G0003
     2,NILE2,MIRE,BIGO,BIG,CIGO,CIG,RTMXX,RTMXY,RTMXZ,RTMYY,RTMYZ,RTMZZ, 2G0004
     3RSUMXX,RSUMXY,RSUMXZ,RSUMYY,RSUMYZ,RSUMZZ,SUMXX,SUMXY,SUMXZ,SUMYY, 2G0005
     4SUMYZ,SUMZZ,PI,SPI,SIGAM,CTGAM,COGAM,COALPH,COBET,CODEL,SIDEL,OA,V 2G0006
     5OL,POW,POW3,PV1,PV2,TE,CS1,CS2,AMP,JIG,XSI1,XSI2,ADD,RATIO,XMU1,XM 2G0007
     6U2,S1,S2,SV1,SV2,SV3,H1,H2,HX1,HX2,HY1,HY2,W1,W2,Z1,Z2,X11,X12,X21 2G0008
     7,X22,Y11,Y12,Y21,Y22,ROMG31,ROMG32,COMG31,COMG32,GP11,GP12,GM11,GM 2G0009
     812,GP31,GP32,GP51,GP52,T11,T12,T21,T22,T31,T32,T41,T42,T51,T52,T61 2G0010
     9,T62,T71,T72,T81,T82                                              2G0011
      DIMENSION C(17)                                                   2G0012
      COMMON C                                                          2G0013
      IF(S1)1,1,2                                                       2G0014
    1 GP31=0.5*SPI                                                      2G0015
      GP51=0.75*SPI                                                     2G0016
      GO TO 9                                                           2G0017
    2 TRY=-PI*S1*S1                                                     2G0018
      T71=SPI*S1                                                        2G0019
      T81=EXPF(TRY)                                                     2G0020
      IF(TRY+3.)5,3,3                                                   2G0021
    3 TERM=-2.*T71                                                      2G0022
      GP11=SPI+TERM                                                     2G0023
      DO 4 II=1,40                                                      2G0024
      A=II                                                              2G0025
      TERM=TERM*TRY*(A-0.5)/(A*(A+0.5))                                 2G0026
    4 GP11=GP11+TERM                                                    2G0027
      GO TO 8                                                           2G0028
    5 X=-3./TRY                                                         2G0029
      SUM=C(1)                                                          2G0030
      DO 7 II=2,17                                                      2G0031
    7 SUM=SUM*X+C(II)                                                   2G0032
      GP11=SUM*T81/T71                                                  2G0033
    8 GP31=0.5*GP11+T71*T81                                             2G0034
      GP51=1.5*GP31-T71*T81*TRY                                         2G0035
    9 IF(S2)11,11,12                                                    2G0036
   11 GP32=0.5*SPI                                                      2G0037
      GP52=0.75*SPI                                                     2G0038
      GO TO 19                                                          2G0039
   12 TRY=-PI*S2*S2                                                     2G0040
      T72=SPI*S2                                                        2G0041
      T82=EXPF(TRY)                                                     2G0042
      IF(TRY+3.)15,13,13                                                2G0043
   13 TERM=-2.*T72                                                      2G0044
```

```
      GP12=SPI+TERM                                                     2G0045
      DO 14 II=1,40                                                     2G0046
      A=II                                                              2G0047
      TERM=TERM*TRY*(A-0.5)/(A*(A+0.5))                                 2G0048
   14 GP12=GP12+TERM                                                    2G0049
      GO TO 18                                                          2G0050
   15 X=-3./TRY                                                         2G0051
      SUM=C(1)                                                          2G0052
      DO 17 II=2,17                                                     2G0053
   17 SUM=SUM*X+C(II)                                                   2G0054
      GP12=SUM*T82/T72                                                  2G0055
   18 GP32=0.5*GP12+T72*T82                                             2G0056
      GP52=1.5*GP32-T72*T82*TRY                                         2G0057
   19 RETURN                                                            2G0058
      END                                                               2G0059
```

APPENDIX B

SUMMATION CONVERGENCE AND ERRORS

The general lattice sums to be evaluated in the program are of the form

$$S_{ij} = C_i \sum_{\substack{\mu_1,\mu_2 \\ =-\infty}}^{\infty} h_i(\mu_1,\mu_2)\phi_1(\mu_1,\mu_2)\left\{\frac{\phi_2(\mu_1,\mu_2)e^{-c_2 h_i}}{1-\phi_2(\mu_1,\mu_2)e^{-c_3 h_i}} + \right.$$

$$\left. + \frac{e^{-c_3 h_i}}{1-\phi_3(\mu_1,\mu_2)e^{-c_3 h_i}}\right\}$$

where C_i is a constant, $h_i(\mu_1,\mu_2)$ is a function of μ_1 and μ_2 which generally increases with increasing μ_1 and μ_2 and ϕ_i is a phase factor of the form $\exp[-2\pi i(c_i\mu_1 + c_i\mu_2)]$. Because of the phase factors it is possible to have a distribution of significant terms over the μ_1-μ_2 plane such as shown in figure 8.

To ensure inclusion of significant terms in such a distribution would require either very complex convergence tests or inclusion of many more terms then required.

To avoid this, the sums were converted to semi-infinite sums over the first quadrant of the μ_1-μ_2 plane. This led to the possible distributions shown in figure 9, where the degree of asymmetry about the μ_1=μ_2 axis depended on the ratio of the lengths of the a_1 and a_2 basis vectors and the angle between them, and the

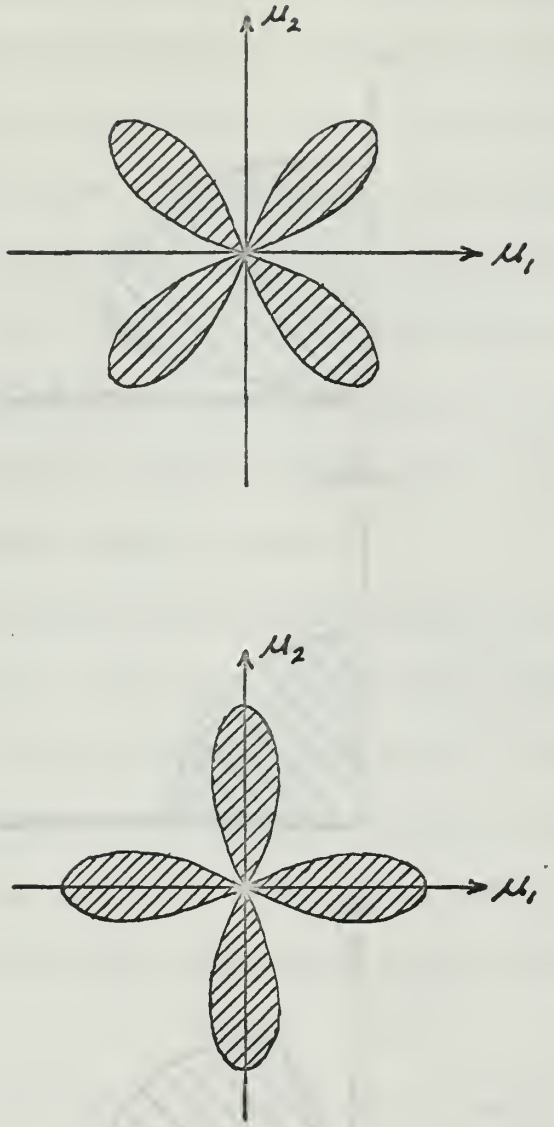


Figure 8: Possible distributions of significant terms of sum over μ_1-μ_2 plane. Shaded area contains all terms of absolute value larger than a given constant.

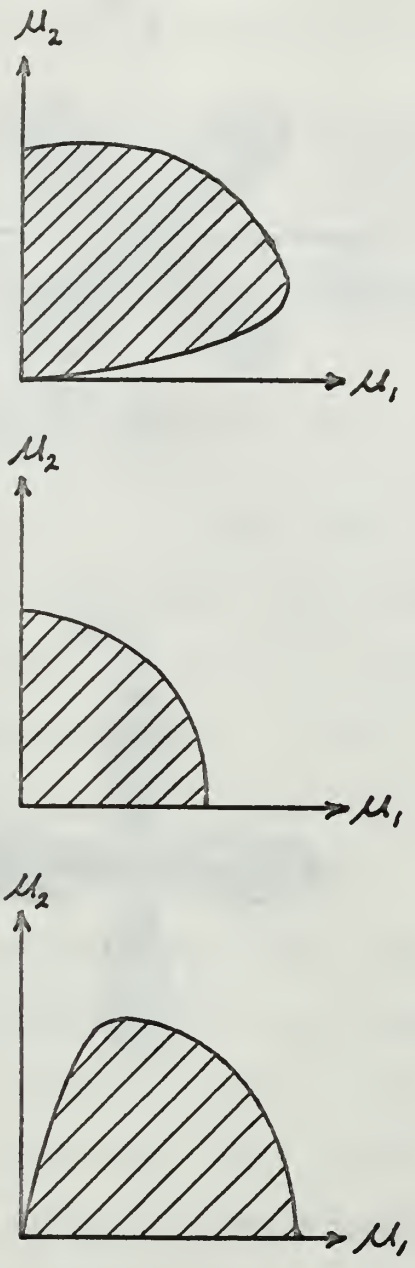


Figure 9: Possible distributions of significant terms of converted sums

particular sum being evaluated, S_{ij}. While these distributions still leave problems in developing convergence tests, the problems are not as formidable as for the original equations.

The solution used in this program proceeded in several steps. First the axial terms, $\mu_1=0, \mu_2=0, 1, 2, 3, \ldots$ and $\mu_2=0, \mu_1=1, 2, 3 \ldots$ were summed together and the convergence test applied to the sum of each pair, $\mu_1=0, \mu_2=i$; $\mu_1=i, \mu_2=0$, until the tests were met for each sum S_{jk}, or N pairs were summed.

The non-axial terms were then treated separately. First a skew factor, $JIG = 2 * MAX\ (\frac{A2}{A1}, \frac{A1}{A2}) \cos\gamma + 1$, was generated. This number is such that the largest term of the sum (in absolute value) must occur at some point within the box $0 \leq \mu_1, \mu_2 \leq JIG$. This was tested against N to ensure $N > JIG$ so that the sums would include the largest term.

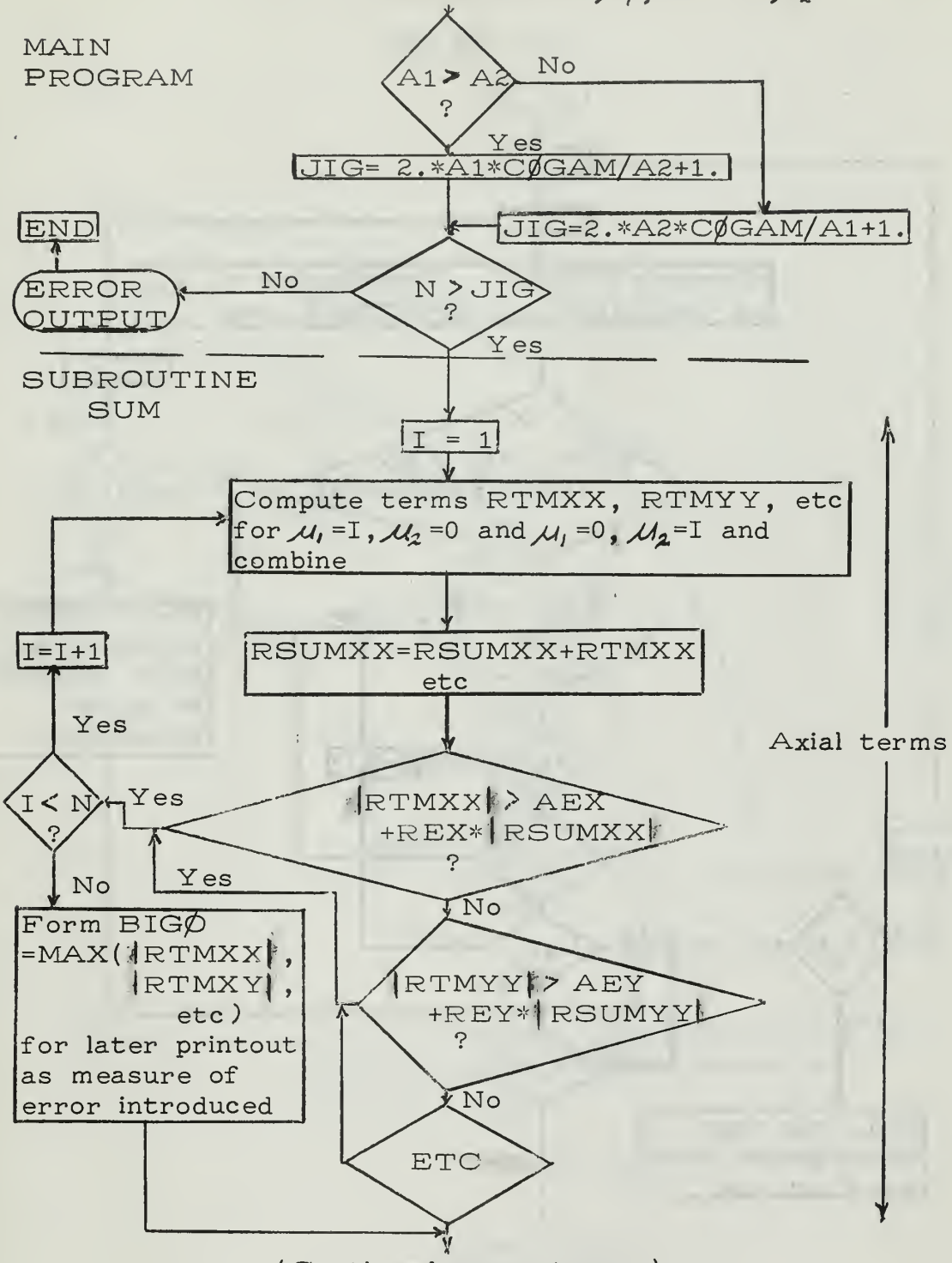
Summing was done by summing all terms $\mu_2 = 1, 2, 3, \ldots$ for $\mu_1=1$ and then for $\mu_1=2$, etc. The convergence test were threefold. First to ensure for given μ_1 that μ_2 assumed all values up to JIG and that this was done for all values of μ_1 up to JIG. This ensured picking up the most significant term of this sum regardless of its magnitude. Second to ensure that for given $\mu_1=a$ if some

term, $\mu_2 \leq a$, did not meet the convergence tests then summing would be done on the pencil $\mu_1=a+1, \mu_2=1, 2, \ldots, a+1$. Last, that summing would not exceed the terms $\mu_1=N, \mu_2=i$; $\mu_1=j, \mu_2=N$, regardless of other tests.

The flow chart for this testing is shown in figure 10. Actual convergence zones for a cubic lattice and a triclinic lattice are shown in figures 11 and 12.

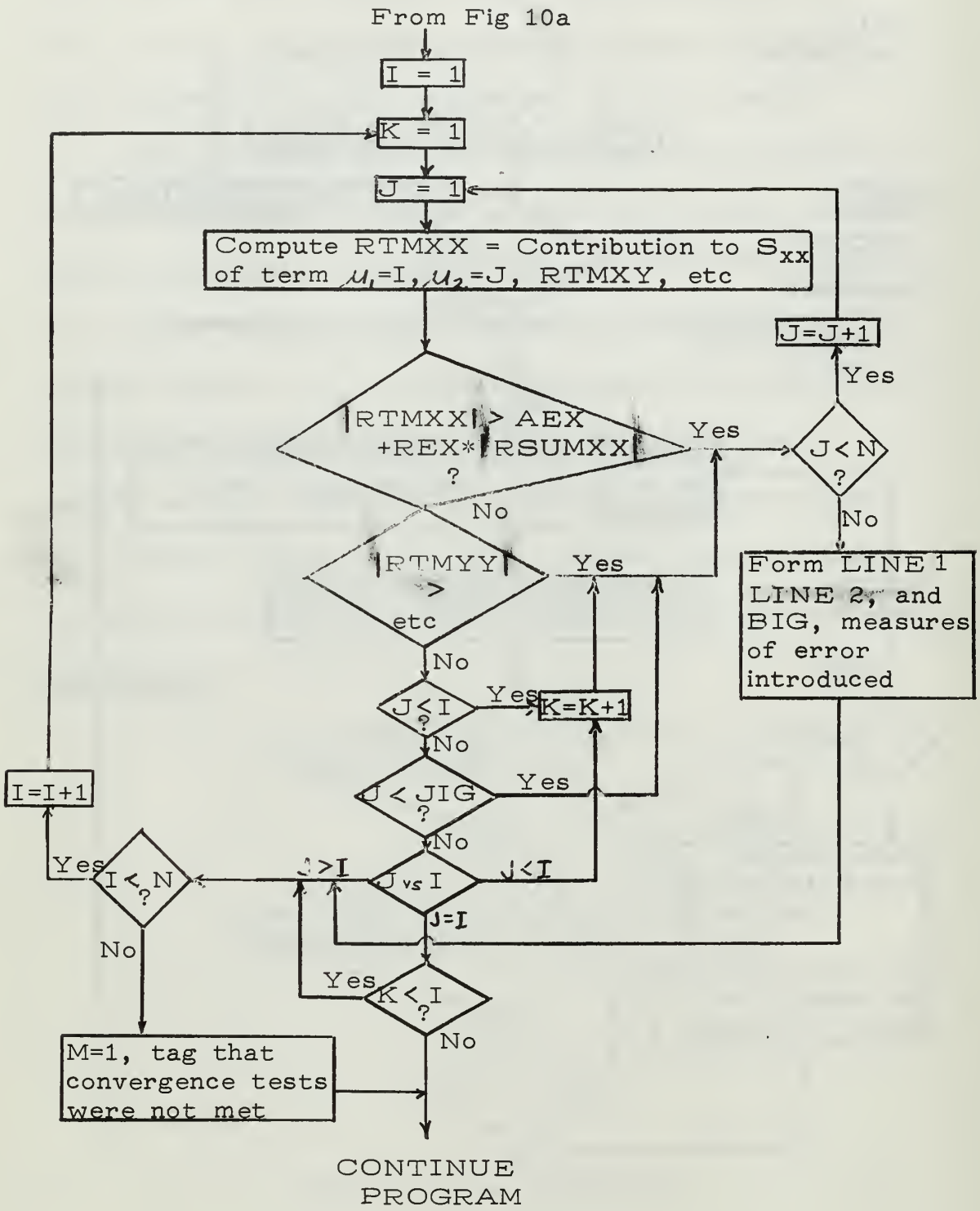
After completing the program it was checked by running sums on 112 lattices (distortions of the basic cubic lattice) for which sums are known from geometric considerations. The error analysis for a relative error limit (REX, etc) of 10^{-4}, 10^{-6}, and 10^{-8} and an absolute error limit (AEX, etc) equal to the relative limit is given in Table 2.

Figure 10a Flow chart of convergence tests common to SUM1-SUM6. Integer variable I refers to values of summing index μ_1, J to μ_2.



(Continued on next page)

Figure 10b Continuation of flow chart



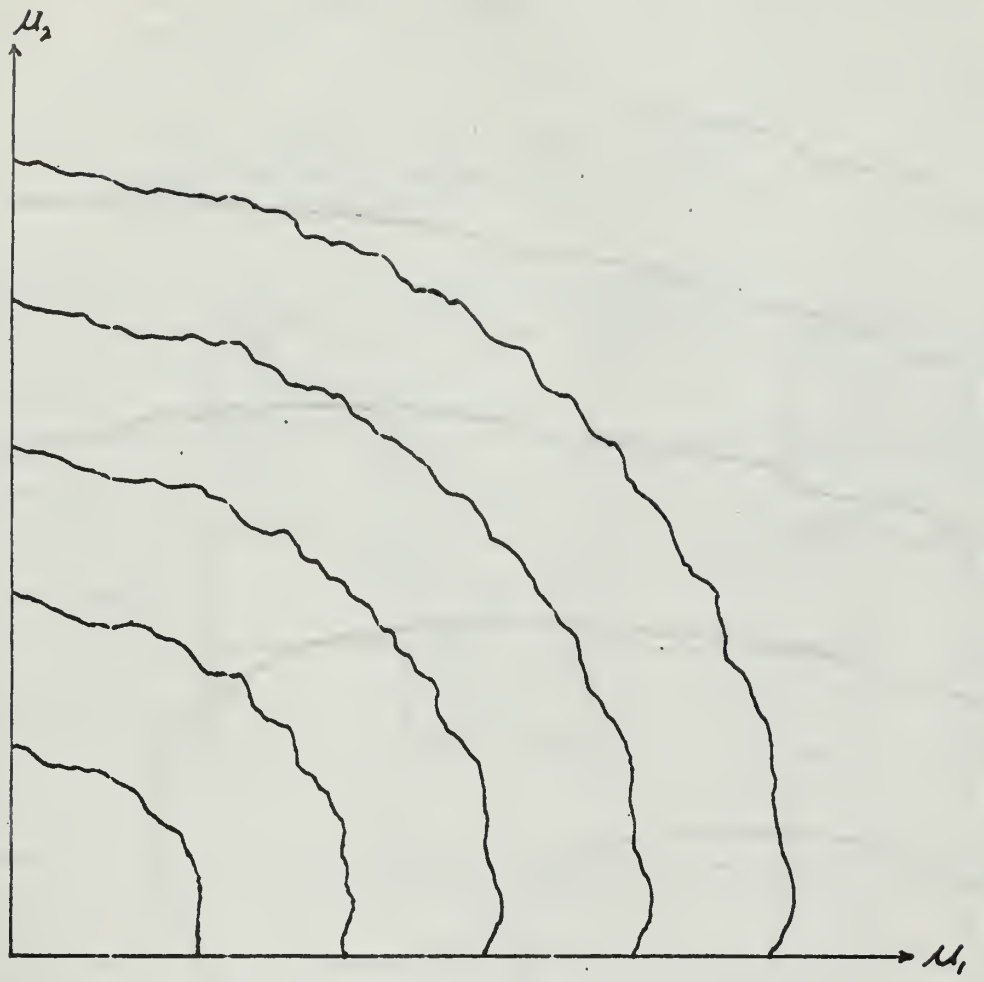


Figure 11: Actual convergence zones plotted for unit cubic lattice using library subroutine CONTOUR.

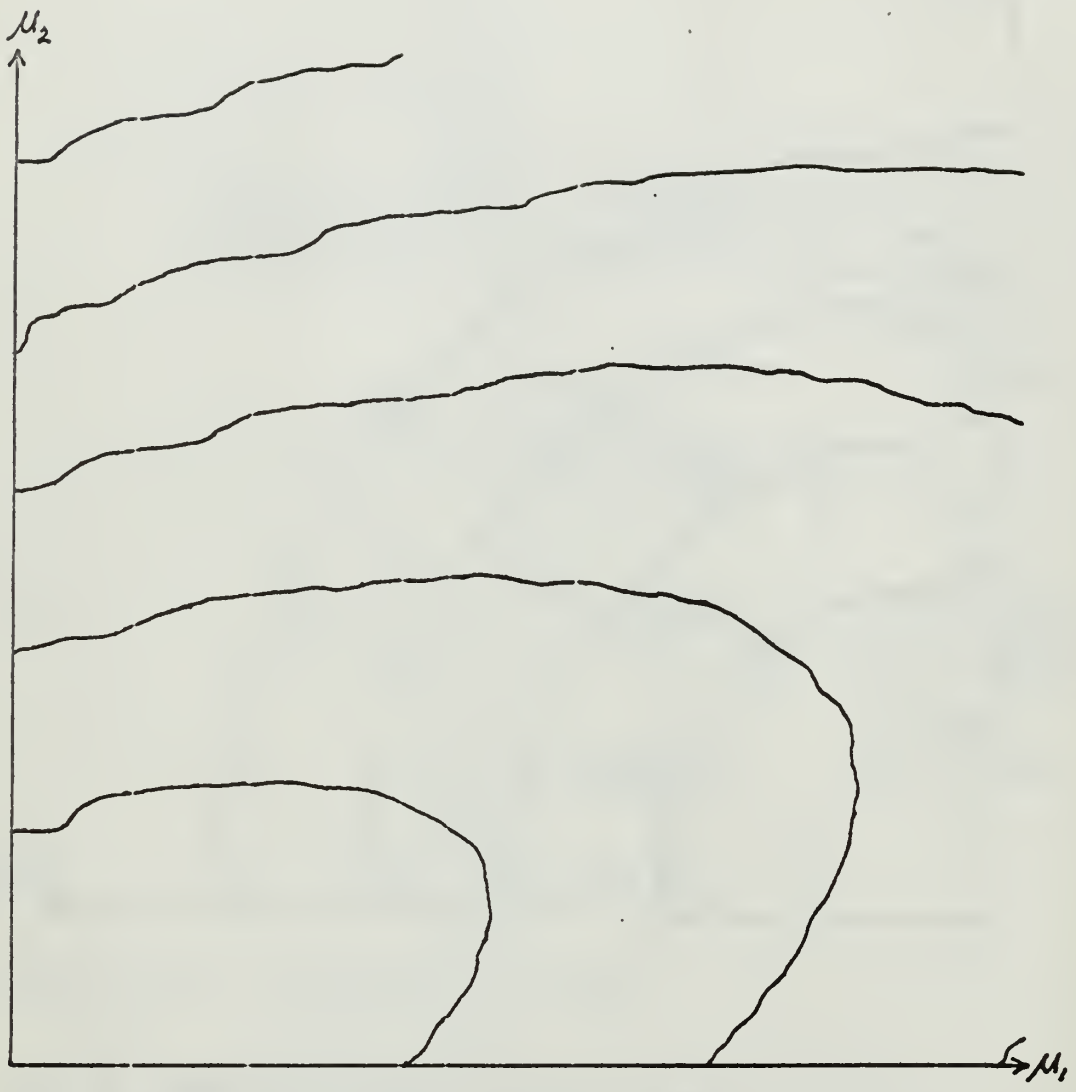


Figure 12: Actual convergence zones plotted for a triclinic lattice using library subroutine CONTOUR.

Table 2: Error analysis of known sums S_{ij}. In each box the left-hand numbers are absolute errors, the right hand numbers are relative errors, the top numbers are maximum values, the bottom are average values, and the center integer is the number of sums evaluated.

2a: Input relative error limit = 10^{-4}
Input absolute error limit = 10^{-4}
All errors X 10^{-6}

Lattice Type	Subroutine Used SUM1	SUM2	SUM3	SUM4&6	SUM5&6
Triclinic	.02 .1 174 .003 .005	0	0	.1 .1 156 .008 .005	0
Monoclinic	.03 .07 12 .004 .01	.1 .2 24 .03 .01	0	.05 .09 8 .008 .01	.04 .06 16 .01 .01
Orthorhombic	0	1. .6 18 .08 .05	0	0	.7 .4 12 .08 .05
Tetragonal	0	.2 .1 54 .07 .06	0	0	.09 .1 36 .003 .009
Trigonal	0	0	0	0	0
Cubic	0	.6 .1 18 .07 .01	0	0	.05 .08 12 .005 .007

2b: Input relative error limit = 10^{-6}
Input absolute error limit = 10^{-6}
All errors X 10^{-8}

Lattice Type	Subroutine Used				
	SUM1	SUM2	SUM3	SUM4&6	SUM5&6
Triclinic	.1 1. 174 .02 .03	0	0	1. 1. 156 .02 .01	0
Monoclinic	.2 .5 12 .06 .1	1. 1. 24 .1 .1	0	.3 1. 8 .05 .2	.2 .09 16 .03 .01
Orthorhombic	0	4. 2. 18 .3 .2	0	0	2. .9 12 .2 .1
Tetragonal	0	2. 1. 54 .1 .1	0	0	.8 1. 36 .04 .03
Trigonal	0	0	0	0	0
Cubic	0	6. .9 18 .4 .07	0	0	.5 .9 12 .05 .1

2c: Input relative error limit = 10^{-8}
Input absolute error limit = 10^{-8}
All errors X 10^{-10}

Lattice Type	Subroutine Used				
	SUM1	SUM2	SUM3	SUM4&6	SUM5&6
Triclinic	.2 1. 174 .04 .03	0	0	.9 1. 156 .04 .02	0
Monoclinic	.1 .4 12 .01 .04	.9 1. 24 .05 .07	0	.1 .8 8 .02 .1	.3 .08 16 .04 .007
Orthorhombic	0	3. 1. 18 .2 .1	0	0	2. 1. 12 .3 .1
Tetragonal	0	3. 2. 54 .06 .05	0	0	1. .9 36 .04 .03
Trigonal	0	0	0	0	0
Cubic	0	7. 8. 18 .4 .5	0	0	.4 .8 12 .1 .07

APPENDIX C

INCOMPLETE GAMMA FUNCTION

In evaluating the lattice sums when the evaluation point lines in the x-y plane an auxilliary convergence function is used to smooth and remove the simple pole of the function being summed. In the equations of Schacher and de Wette this introduces the following four terms into the sums:

$\Gamma(-1/2, \pi h^2)$
$\Gamma(1/2, \pi h^2)$
$\Gamma(3/2, \pi h^2)$
$\Gamma(5/2, \pi h^2)$

where $h=h(\mu_1, \mu_2)$; μ_1, μ_2 summing indices; and

$\Gamma(a,x) \equiv \int_x^\infty t^{a-1} e^{-t} dt$ the incomplete gamma function.

In order to develop a usable program based on Schacher and de Wette's equation it was necessary to obtain a simple subroutine for evaluating these functions repeatedly as h changed with μ_1 and μ_2. Unfortunately incomplete gamma functions are not widely used and the only subroutines available from other sources were those designed to tabulate Γ (a, x) over a wide range of values of a and x. Since Γ (a, x) is a transcedential whose "best" approximation is

an assymptotic series, tabulating programs are both cumbersome and slow.

Three possibilities were considered for this program. First, adapt one of the existing programs for limited use. This was tried but even after abstracting the desired parts from the best of these programs we were left with a double-precision program with an evaluation time, per h value, of about 0.5 sec. Since we contemplated hundreds of thousands of evaluations per lattice we ultimately discarded this approach.

The second possibility considered was simply storing tabulated values over the range h=0-100 and interpolating as necessary. However to obtain program accuracies of $\pm 10^{-9}$ for S_{ij} would have required storing 4000 or more values. This, added to the large program storage already generated would have overflowed the internal storage of all but the largest computers available. Tape or disc storage would again increase run time too much so this approach was also discarded.

The final possibility was adopted, that of formulating new approximations to the incomplete gamma function. Ultimately a set of power series approximations was developed,

using the Tau Method of Lanczos,[7] to span the range $\pi h^2 = 3-\infty$. Another, long-known series, well convergent for small values of x, was used in the range $\pi h^2 = 0-3$

The expansions are

$$\Gamma(1/2, x) = \begin{cases} \sqrt{\pi} - 2\sum_{k=0}^{40} \frac{(-1)^k \sqrt{x}\, x^k}{k!(k+1/2)} & 0 < x \leq 3 \\ \left(\frac{3}{x}\right)^{17} \sum_{k=1}^{17} C_k \left(\frac{x}{3}\right)^k & 3 < x \end{cases}$$

where the $C_{k's}$ were generated using the Tau Method. The other functions, $\Gamma(3/2, x)$, etc were obtained from $\Gamma(1/2, x)$ by using the recursion relation $\Gamma(a+1, x) = a\Gamma(a, x) + x^a e^{-x}$.

The Tau Method is well adopted to exploring several possibilities of approximating series on the computer. In this instance we examined a total of 240 possibilities, combining the four a values, $-\frac{1}{2}$, $\frac{1}{2}$, $\frac{3}{2}$, $\frac{5}{2}$ with 3 possible ranges of approximation, $\frac{1}{2} < x$, $1 < x$, $3 < x$ and in each case examining series of 2, 3, 4 ..., 21 terms. In general, accuracy increased with increasing a value, increasing end point b, $b < x$, and increasing number of terms in the series. We used $a = \frac{1}{2}$ vice $\frac{3}{2}$ or $\frac{5}{2}$ because it matched the a value of

[7] Lanczos, C., Applied Analysis, 464-485, (Prentice Hall, Englewood Cliffs, N.J., 1961)

the expansion for $0 < x \leq 3$. A 17 term series was used since it exhausted machine accuracy of the computer used ($\pm 10^{-11}$), and any higher series would add no accuracy.

Having settled on an approximation it was checked against a double precision routine known to be accurate to $\pm 10^{-11}$. The graph of the error of the approximation is shown in figure 13.

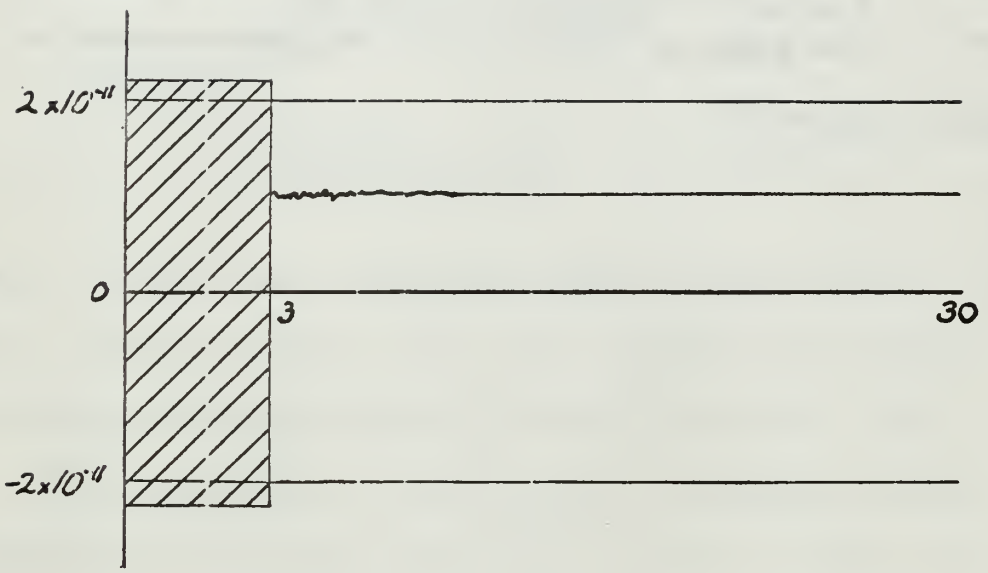


Figure 13: Error curve for Incomplete Gamma Function approximation. Abscissa is x, ordinate is $\Gamma^*(1/2,x)-\Gamma(1/2,x)$ where Γ^* is approximation and Γ is actual value of Incomplete Gamma Function. Shaded area represents an oscillation of error of such a high frequency that it could not be faithfully represented on this scale.

APPENDIX D

APPLICATION TO BENZENE

During the preparation of this program R.M. Hexter of the Mellon Institute suggested an application to a long-standing problem in molecular spectroscopy. This work has been completed and is detailed below as an example of applying the program to an actual problem.

In calculating the electronic spectrum of benzene it is necessary to compute the transition moments of the free molecules. These moments depend on the dipole-dipole sums of the crystal. Various workers computing these sums by various methods have obtained varying values for the sums. Craig and Walsh[8] have set out the crystalline structure assumed and tabulated the values obtained by two summation procedures. This program was used to check these values with results tabulated below.

The benzene crystal model consists of an orthorhombic unit cell with four molecular orientations at the corners and faces. If we superimpose cartesian reference frames on each molecule we can identify our molecules as follows:

[8]D. Craig and J. Walsh, J. Chem Soc 1958, 1613

Molecular Type	Unit Cell Location	Crystal Axis	Direction Cosines x	y	z
I	0,0,0	a	.6365	-.2992	.7109
		b	.2000	.9541	.2229
		c	-.7450	0	.6671
II	$\frac{1}{2},0,\frac{1}{2}$	a	-.6365	.2992	-.7109
		b	-.2000	-.9541	-.2229
		c	-.7450	0	.6671
III	$0,\frac{1}{2},\frac{1}{2}$	a	-.6365	.2992	-.7109
		b	.2000	.9541	-.2229
		c	.7450	0	.6671
IV	$\frac{1}{2},\frac{1}{2},0$	a	.6365	-.2992	.7109
		b	-.2000	-.9541	-.2229
		c	.7450	0	-.6671

Where (a,b,c) forms the cartesian frame of the unit cell. The unit cell parameters are (at -3° C)

$a_1 = 7.460$ Å $\qquad \alpha = \beta = \gamma = 90°$

$a_2 = 9.666$ Å

$a_3 = 7.034$ Å

The problem then is to compute the interaction energy of a unit dipole in the i- direction in molecule I due to a lattice of unit dipoles in the j-direction in molecules of type ν, where i, j = x, y, z; ν = I, II, III, IV.

In comparing figures obtained by this program with those tabulated by Craig and Walsh two difficulties arise. First dipole-dipole energies from this program work out in recipricol angstroms per coulomb squared while Craig and

Walsh tabulate in recipricol centimeters (wave number) per electronic charge squared. This requires multiplying the results of this program by 1.161×10^5 to be comparable.

Second Craig and Walsh assume an infinite spherical crystal while this program assumes an infinite slab-shaped crystal. Thus depolarization factors must be applied. The two systems are:

Sperical	Slab-shaped
$E_{xx} - \frac{4\pi}{3Vol}$	$E_{xx} + 0$
$E_{yy} - \frac{4\pi}{3Vol}$	$E_{yy} + 0$
$E_{zz} - \frac{4\pi}{3Vol}$	$E_{zz} - \frac{4\pi}{Vol}$

Thus, to be comparable we must add $-(4\pi/\text{vol}) = 0.0165170$ to zz terms generated by this program and subtract $-(4\pi/\text{vol}) = 0.0082585$ to xx and xy terms generated by this program. (Where vol = volume of unit cell in Å)

GENERAL PROCEDURE

With these considerations in mind the computation becomes straight-forward if tedious. First we will compute electric field components at molecule I along the crystal axes a, b, c due to an assumed set of unit dipoles along the a, b, and c axes at molecular positions I, II, III, and

IV. This is done by calculating the field at the appropriate position of molecule I (given by XJI, XJ2, XJ3) within each of the I, II, III, and IV sublattice unit cells. Then we correct the depolarization factors and apply the conversion factor. Then, using the direction cosines of the type I molecule for each molecular axis x, y, and z (with respect to the a, b, c axes) we can get the x, y, and z components of field at I due to a, b, and c dipoles at all molecular positions. Then by multiplying by the direction cosines for each molecule respectively we get energies of the x, y, and z dipoles of molecule I due to x, y, and z dipoles at each molecular position. These we compare with similarly tabulated results of Craig and Walsh.

DETAILS OF COMPUTATION

To get the a, b, and c field components at molecule I we enter the program with:

A1 = 7.460	XALPH = 90.
A2 = 9.666	XBET = 90.
A3 = 7.034	XGAM = 90.
	XDEL = 0.

$AEX=REX=AEY=REY=AEZ=REZ=10^{-7}$

N=20

and for various molecules:

	I	II	III	IV
XJ1	0	½	0	½
XJ2	0	0	½	½
XJ3	0	½	½	0

Since the crystal is orthorhombic we get $S_{ij}=0$, $i \neq j$. The three nonzero outputs SUMXX, SUMYY, and SUMZZ here correspond to the a, b, and c field components. The computed S_{ij} values, depolarization correction, conversion factor, and converted values are listed below:

Fields at I due to molecules of type	i-field component due to j-dipoles	Computed Values	Depolarization	Corrected Values
I	aa	.0104233	-.0082585	.0021648
	bb	.0011720	-.0082585	.0070865
	cc	.0115953	.0165170	.0049217
II	aa	.0240220	-.0082585	.0157635
	bb	-.0187985	-.0082585	-.0270570
	cc	-.0052235	.0165170	.0112935
III	aa	-.0055470	-.0082585	-.0138055
	bb	.0231906	-.0082585	.0149321
	cc	-.0176436	.0165170	-.0011266
IV	aa	.0080050	-.0082585	-.0002535
	bb	.0209184	-.0082585	.0126599
	cc	-.0289234	.0165170	-.0124064

Molecule	Axes	Corrected Value	Conversion Factor	Converted Values
I	aa	.0021648	1.161×10^5	251.333
	bb	-.0070865		-822.742
	cc	.0049217		571.409
II	aa	.0157635		1830.142
	bb	-.0270570		-3141.317
	cc	.0112935		1311.175
III	aa	-.0138055		-1602.818
	bb	.0149321		1733.616
	cc	-.0011266		-130.798
IV	aa	-.0002535		-29.431
	bb	.0126599		1469.814
	cc	-.0124064	1.161×10^5	-1440.383

Now we need the x, y, and z components of these fields at molecule I; I-I (x, m), I-I (y, m), I-I (z, m), etc (m=a,b,c). Here we need the molecule I direction cosines for x, y, or z with respect to a, b, and c. Two examples suffice:

x - field components

Fields at I due to dipoles at	Unit Call Component	Value	Dir. Cos	Molecular Component
I	aa	251.333	.6365	159.9734
	bb	-822.742	.2000	-164.5484
	cc	571.409	-.7450	-425.6997
II	'			
'	'			
'	'			

y - field components

Fields at I due to dipoles at	Unit Call Component	Value	Dir Cos	Molecular Component
'				
'				
'				
II	aa	1830.142	-.2992	-547.5784
	bb	-3141.317	.9541	-2997.1305
	cc	1311.175	0	0
III				
'				
'				

From these we can make up the energies by multiplying the molecular components by the direction cosines of the source dipole at the molecular position of interest.

Since we have tabulated the molecular components I-I (x, m) and I-II (y, m), if we want the energy of an x-dipole in molecule I due to a lattice of y-dipoles at position I, I-I (x,y), we need only multiply the molecular components I-I (x, m) by the y direction cosines of type I and sum. We show the computation of I-I (x,y) and I-II (y,z) below:

Field Component	Axis	Value	Direction Cosine	Energy Contribution
			Iy dipoles	
I-I (x,)	aa	159.9734	-.2992	-47.8640
	bb	-164.5484	.9541	-156.9956
	cc	-425.6997	0	0
			I-I (x,y) energy	-204.8596
			IIz dipoles	
I-II (y,)	aa	-547.5784	-.7109	389.2734
	bb	-2997.1305	-.2229	668.0603
	cc	0	.6671	0
			I-II (y,z) energy	1057.3337

These then are the numbers to be compared with those tabulated by Craig and Walsh. Their table contains numbers obtained both from the Ewald-Kornfeld[9] method applied to an infinite sphere and from a direct molecule-molecule summation over a sphere of radius 20 A. The comparison is shown below. Results (a) are from this program, (b) from the Ewald-Kornfeld method, and (c) from direct molecule-molecule summation.

[9] Kittel, Introduction to Solid State Physics, 2nd Ed, 347, (John Wiley and Sons, Inc., New York, 1954)

Dipole Axes	Results	Molecule Sites I, I	I, II	I, III	I, IV
x, x	(a)	-386.06	-111.94	-791.29	-728.72
	(b)	-386	-112	-791	-729
	(c)	-415	-92	-769	-771
y, y	(a)	726.45	-2695.73	-1721.61	1340.62
	(b)	727	-2679	-1723	1341
	(c)	790	-2629	-1713	1405
z, z	(a)	-340.47	185.49	-954.10	-553.20
	(b)	-341	185	-955	-553
	(c)	-375	220	-950	-587
x, y	(a)	204.86	-947.96	-25.57	274.87
	(b)	205	-947	-25	275
	(c)	233	-934	-8	289
x, z	(a)	206.94	1339.72	-737.54	794.70
	(b)	207	1340	-738	795
	(c)	181	1306	-818	833
y, z	(a)	228.43	-1057.33	-27.76	306.32
	(b)	228	-1058	-27	307
	(c)	260	-1041	-7	323

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3. REPORT TITLE

A COMPUTER PROGRAM FOR EVALUATING LATTICE SUMS

4. DESCRIPTIVE NOTES (Type of report and inclusive dates)

THESIS

5. AUTHOR(S) (Last name, first name, initial)

DICKMANN, David B.

6. REPORT DATE	7a. TOTAL NO. OF PAGES	7b. NO. OF REFS
22 April 1966	82	9

8a. CONTRACT OR GRANT NO.	9a. ORIGINATOR'S REPORT NUMBER(S) 1
b. PROJECT NO. N/A	
c.	9b. OTHER REPORT NO(S) (Any other numbers that may be assigned this report)
d.	

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A recurring problem in solid state physics is that of determining the electrostatic field or potential at a point within the crystal lattice arising from the molecules of the lattice themselves. A typical problem is that of finding the electrostatic binding potential of an ionic lattice assuming point charges.

Nijboer, de Wette and others have worked toward perfecting a method for calculating the electric field arising from a lattice of dipoles. This work culminated in a paper by de Wette and Schacher detailing a procedure which ensures a rapidly converging summation of the three dimensional lattice sums involved.

The present paper is an extension of the latter, presenting a computer program for evaluating dipole fields in a crystal lattice using the equations obtained by de Wette and Schacher.

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